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Principal Investigator Dr. Martin R. Flannery

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in Atomic Molecular Gases

Project No: G-41-631

Project Director: Dr. Martin R. Flannery

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G-41-631

REPORT: Quarterly R&D Status Report
covering the period October 8, 1973 - January 8, 1974

PROJECT-TITLE: Calculation of Electron Impact Cross Sections
from Metastable States in Atomic and Molecular Gases

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ABSTRACT

An account of the research carried out in the period 8 October 1973 - 8 January 1974 is presented. Available data on electron-excited atom collisions is referenced and theoretical methods are evaluated. Calculation of the $2^1,3S - 2^1,3S, 3^1,3S, 3^1,3P, 3^1,3D, 4^1,3P$ transitions in helium by electron impact are provided by using the Born and Ochkur approximations up to 1000 eV impact energy. Measured cross sections for the ionization of metastable helium, neon and argon are also given.

1. Available Data on Electron-excited Atom Collisions

A review of all the various theoretical approaches applicable to electron-excited atom collisional excitation and ionization was initiated and is now well underway. In general, all of the available theories have been applied to e-H(1s) and e-He(1s²) excitation collisions, while only the simpler theories (e.g. the Born approximation) have been applied to excitation of more complex atoms from their ground-state. For ionization of ground-state atoms, only the Born (and related) approximations and classical treatments have been applied.

While there have been literally hundreds of investigations reported in the literature concerning collisions involving ground-state species, there are only several reports on electron collisions with atoms initially in a prepared excited state. These investigations are limited only to metastable helium and are as follows:

(a) Excitation (Theoretical Calculations)

- (1) "The Conversion of Metastable Helium from the Singlet to the Triplet State by Electron Collision".

R. Marriott, Proc. Phys. Soc. A 70, 288 (1957).

Method: close-coupling approximation. Transitions $2^1S - 2^3S$

- (2) "The $2^3S - 2^3P$, 3^3P , 3^3D , 4^3D excitations of helium atoms by electrons".

B. L. Moiseiwitsch, Mon. Not. Roy. Astron. Soc. 117, 189 (1957).

Method: Born Approximation

- (3) "Excitation of helium from the 2^3S state by electron collision"

V. I. Ochkur and V. F. Bratsev, Soviet Astronomy 9, 797 (1966).

Method: Ochkur approximation. Transitions $2^3S - n^{3,1}L$, $n = 3, 4, 5, 7, 10$

- (4) "Low-energy electron scattering by metastable helium".

R. Marriott, Proc. Phys. Soc. 87, 407 (1966).

Method: Close-coupling approximation. Transitions $2^{1,3}S - 2^{1,3}S, 3^{1,3}S$

- (5) "Excitation of Triplet states in helium by electron impact".

D. J. T. Morrison and M. R. H. Rudge, Proc. Phys. Soc., 91, 565 (1967).

Method: Rudge-Ochkur approximation. Transitions $2^1S - 2^3S$.

- (6) "Generalized Oscillator Strengths of the Helium Atom".

Y. K. Kim and M. Inokuti, Phys. Rev. 181, 205 (1969).

Method: Born approximation. Transitions $2^1S - 2^1P, 2^3S - 2^3P, 3^3S, 3^3P, 3^3D$

- (7) "Low-energy Scattering of electrons by helium".

P. G. Burke, J. W. Cooper and S. Ormonde, Phys. Rev. 183, 245 (1969).

Method: Close-coupling approximation. Transitions $2^{1,3}S - 2^{1,3}P$

- (8) "Inelastic Scattering of Electrons by Helium".

R. S. Oberoi and R. K. Nesbet, Phys. Rev. A 8, 2969 (1973).

Method: Close-coupling approximation. Transitions $2^1S - 2^{1,3}S, 2^{1,3}P$.

(b) Ionization (Theoretical Calculations)

- (1) "Calculations of Absolute Ionization Cross Sections of He, He^{*}, He⁺, Ne, Ne^{*}, Ne⁺, Ar, Ar^{*}, Hg, and Hg^{*}".

L. Vriens, Phys. Letters, 8, 260 (1964).

Method: Classical (Gryzinski)

- (2) "Total Cross Sections for Inelastic Scattering of Charged Particles by Atoms and Molecules".

J. S. Briggs and Y. K. Kim, Phys. Rev. A, 3, 1342 (1971).

Method: Bethe approximation (Asymptotic-Born)

(c) Ionization (Experimental)

- (1) "Electron Collisions with atomic and molecular oxygen".

W. L. Fite and R. T. Brackmann, Proceedings of the Sixth International Conference on Ionization Phenomena in Gases, Paris, 1963, edited by P. Hubert and E. Cremion-Alcan (S.E.R.M.A., Paris, 1964) vol. 1. p. 21.

- (2) "Excitation to the Metastable States and ionization from ground and metastable states in helium".

L. Vriens, T. F. M. Bensen, and J. A. Smit, Physica, 40, 229 (1968).

- (3) "Electron-Impact Ionization of He(2s ³S)".

D. R. Long and R. Geballe, Phys. Rev. A 1, 260 (1970).

- (4) "Ionization of metastable rare gas atoms by electron impact".

A. J. Dixon, M. F. A. Harrison and A. C. H. Smith: Abstracts of Papers (VIII ICPEAC, Beograd, 1973) p. 406.

- (5) "Electron Impact Excitation-Ionization of N₂ metastables".

P. D. Tannen, A. Garscadden and M. L. Lake, Bull. Amer. Phys. Soc. 18, 1506 (1973).

2. Evaluation of Theoretical Methods

In the absence of firm theoretical and experimental studies of electron-excited atom collisions, it is very difficult to select a particular theory that is most suitable to the needs of the present investigation. Generally, the goodness of any particular theoretical approach is guided largely by its comparison with experiment and with other theories. Moreover, even for excitation from the ground-state, the problems relating to the excitation of atoms by electrons at low and intermediate impact energies remain as yet largely unresolved. For excited-state systems information is scarce and one has to look to data on excitation from ground-state systems - the physics of which

being significantly different from that of excited states. One has also to be in a position to apply various theories to the excited state problem in order to make progress.

During the past three months, five main methods (together with their derivatives) have been considered for excitation:

- (1) The quantal close-coupling method
- (2) The Born and Born-Ochkur approximations
- (3) The Vainshtein, Presnyakov and Sobelman approximation
- (4) The semiclassical close-coupling method
- (5) The polarized orbital distorted wave model.

(a) Evaluation of the Close-Couplings Method

In (1), the total wavefunction for the colliding (e-x) system is decomposed into partial waves by means of an expansion based on the unperturbed atomic wavefunctions. The incident electron's motion is coupled to the electronic motions of the atomic target. This method has been applied to a limited number of systems over a limited range of impact energies (generally between the first and second excitation thresholds). In general, such calculations require a considerable expenditure of computer time with the computational labor increasing extremely rapidly as the number of target states are increased. Even with this additional labor calculations of this type do not yield a corresponding improvement in the results.

While the method has been successful in predicting the shapes and widths of resonances at very low impact energies (between various excitation thresholds) it has been markedly less than successful in providing accurate cross sections (when compared with experiment). For example for impact energies between 10.2 eV

and 12.1 eV (the $n = 2$ and $n = 3$ excitation thresholds for $H(1s)$) the $1s - 2s$ and $1s - 2p$ calculated cross sections¹ are in reasonably good agreement with experiment² while for energies above the $n = 3$ threshold, the approximation fails badly. Moreover, Burke and Taylor³ carried out a very refined close-coupling calculation including correlation for the excitation of $He^+(1s)$ to $He^+(2s)$ by electrons with energy in the range from threshold if 40.8 eV to 46 eV and the computed cross sections are a factor of two larger than the very recent accurate experimental values of Peart and Dolder⁴. The close coupling method has not been applied to excitation of complex atomic systems from the ground state at intermediate energies.

Even aside from the fact that the quantal close coupling method fails at intermediate energies, its application to e-excited complex atomic systems is impractical. The number of closely lying excited states that require coupling with the relative motion is so much greater than the number involved with excitation from the ground state. Given a near infinite amount of computer time, one unfortunately could not place much reliance on the calculated cross sections for even the $2^1S - 3^1P$ transition in helium.

In an effort to remove some of the defects inherent in the close-coupling method, a modification - the pseudo-state expansion - has been recently proposed. This modification essentially is an artificial injection of unphysical states designed to take full account of the polarization attraction present in e-atom collisions. Up to the present it has only been applied to $e-H(1s)$ and $e-He^+(1s)$ collisions and numerical agreement with experiment is somewhat improved but an incorrect cross section shape is obtained. Before, however, the pseudo-state expansion method can be employed for the simple atomic systems, the nature of convergence of the pseudo-state method must be fully explored for $e-H(1s)$,

$e\text{-He}^+(1s)$ and $e\text{-He}(1s^2)$ collisions. Since the method is an extension of the quantal close-coupling method, its application is even more horrendous and hazardous and it is still not clear how well this method converges to accurate total cross sections when a truncation is employed.

(b) Evaluation of the Born Approximation for Excited States

The question of the limits of validity of the Born approximation to inelastic collisions is by no means simple. It can be shown that the approximation is clearly applicable at high electron speeds v when the inequality $e^2/\hbar v \ll 1$ is fulfilled. This general condition does not contain any specific characteristics of the transition under examination, and, in principle, can be sufficient but not necessary. Sobelman suggests that $E/\Delta E \gg 1$ where E is the incident energy and ΔE the excitation energy is an appropriate condition. This condition yields the previous condition for excitation from ground states. It is very important to note that for transitions between excited states for which ΔE is not large the Sobelman condition can also be fulfilled when $\frac{e^2}{\hbar v} \sim 1$ and even when $\frac{e^2}{\hbar v} > 1$.

The question then arises whether one can in this case use with confidence the Born approximation to provide a reliable estimate of the cross section. It is impossible at this time to seek the answer from theory; and reliable experimental data is available only for transitions from the ground state. However, there is some indirect experimental evidence-obtained from spectral line broadening-that yields useful information on the Born approximation when applied to optically allowed transitions. This indirect experimental data shows that the Born approximation yields good results in many cases.

It is therefore very appropriate at this stage to apply the Born approximation to e -metastable rare gas atoms. The results would be extremely useful and valuable not only by providing a handle on the cross sections but also in

laying the foundations to a systematic investigation of e-excited atom collisions.

Moreover, simple modifications to the Born approximation can be readily carried out e.g. Ochkur has proposed an ingenious method by which electron-exchange can be incorporated into Born's approximation and in general this modification has lead to better agreement with experiment for e-H(1s) and e-He(1s²) collisions. Also a "normalized" Born calculation which does not violate probability conservation can be carried out.

(c) Physics of the e-excited Atom Collision

In the close coupling method, Born's approximation and other related methods based on the expansion of the total wave function for the collision system in terms of unperturbed atomic states, the interaction between the electron and the atom is treated as a perturbation. Here the averaged attraction of the incident electron to the screened nucleus is of primary significance and any details of the repulsion of the atomic electrons are explicitly ignored. For weak interactions with ground-state systems and particularly for closed-shell systems this is reasonable. However, when an atom is initially in an excited state, the electron is generally quite distant from the core (for H(n), $r_1 = n^2 a_0$, for He(1s 2¹S) $r_{12} = 5.3 a_0$, $a_0 = .529 \cdot 10^{-8}$ cm.). Therefore, the incident electron is subjected, not to the averaged field of the orbital electron about the core and the nuclear core, but actually to two strong Coulombic fields - to the e-e repulsion and to the e-core attraction. Penetrating close encounters are of prime importance. The combination of these two fields to result in an averaged field is good only for distant encounters. For the close encounters that are important in the present context, one must seek such methods which solve

the problem by taking the repulsion of the electrons specifically into account together with e-core attraction even in the first approximation.

The approach proposed by Vainshtein, Presnyakov, and Sobelman⁶ is the only quantal treatment available that attempts to do this. The method has been remarkably successful for both e-H(1s) and e-He(1s²) excitation and ionization collisions, but has not yet been explored for e-excited atom collisions. However, there remains some unresolved mathematical difficulties associated with the various approximations the authors made in arriving at their final expression for the cross sections. The method can take account of electron-exchange and is definitely of sufficient interest so as to warrant actual calculations on electron-excited atom systems.

(d) The Semiclassical Close Coupling Approximation

In this method^{7,8}, the motion of the incident electron is separated from the motion of the target electrons by using the JWKB approximation, and the atomic states of the target are closely coupled. Thus details of the target are furnished by quantum mechanics while the incident electron is described semi-classically. The basic method has many derivatives (Eikonal, Impact Parameter, Glauber approximations etc.). Its success with e-H(1s) and e-He(1s²) collisions is remarkable and is sufficiently promising to deserve attention for e-excited atom collisions.

(e) Polarized Orbital Distorted Wave Model

McDowell et al.⁹ have only recently reported a method which apparently yields cross sections for e-H(1s) and e-He⁺(1s) excitation collisions in remarkable harmony with the experimental data^{2,4} in the low and the intermediate energy range. Its possible extension and applicability to excited complex systems is at present under consideration..

The above evaluation (a) - (e) indicates what I now consider to be the best line of approach. In the absence of firm theoretical and experimental data

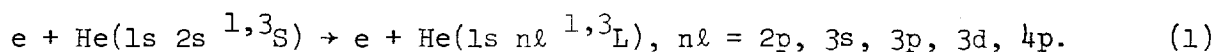
on electron-excited atom collisions which would have helped the selection of a theory, the most sound approach is to actually carry out calculations using several different theories for the e-He^{*} system as a test; the amount of agreement or disagreement between the theories providing valuable insight into the physics of the problem, and hopefully, experimental data will become available during the course of this investigation.

3. Ionization of Metastable Rare Gas Atoms

At the Belgrade conference (July 1973), Dixon et al. presented preliminary experimental data on the ionization of metastable rare gas atoms by electron impact - He, Ne and Ar. They produced the metastables by charge exchange of parent ions in caesium. Unfortunately, they did not have a very good knowledge of the fraction of neutral atoms that were excited or the fraction in each of the lower metastable levels. They assumed 81% helium metastable (mainly triplet), 50% metastable neon, 20% metastable argon. These percentages are subject to considerable uncertainty. Their derived cross sections, however, are in substantial agreement with those obtained from a classical Gryzinski formula. The shape of their helium data to 20 eV agrees with Fite and Brackman while the absolute magnitude at the maximum agrees with Long and Geballe. Dr. Dixon¹⁰ has kindly supplied me with his experimental data (well prior to publication) which are reproduced for your interest in figs. 4-6.

4. Theoretical Calculations Completed in First Quarter

In order to begin a systematic investigation of e-excited atom collisions, and in keeping with the discussion (b), we have applied the Born approximation and the Ochkur Approximation (which takes account of electron exchange) to the following processes,



The cross section formula given by Born's approximation is (in atomic units)

$$Q_{if}^B(v_i) = \frac{8\pi}{v_i} \int_{v_i - v_f}^{v_i + v_f} |F_{if}(K)|^2 \frac{dK}{K^3} \quad (2)$$

and, according to Ochkur's approximation is given by

$$Q_{if}^{S_O S}(v_i) = \frac{2\pi}{v_i} \int_{v_i - v_f}^{v_i + v_f} \left[4 \left(1 - \frac{K^2}{v_i^2} \right) \delta_{S_O S} + (2S + 1) \frac{K^4}{v_i^4} \right] |F_{if}(K)|^2 \frac{dK}{K^3} \quad (3)$$

S_O, S = singlet 1 or triplet 3,

where

$$F_{if}(K) = \langle \phi_i(r_1, r_2) | \sum_{i=1}^2 e^{ik \cdot r_i} | \phi_f(r_1, r_2) \rangle \quad (4)$$

is the generalized form factor connecting the initial helium electronic state with wavefunction $\phi_i(r_1, r_2)$ to the final electronic state with wavefunction $\phi_f(r_1, r_2)$. The speed of the projectile electron is v_i (a.u.) before the collision and v_f (a.u.) after the collision and $K = v_i - v_f$ is the momentum change. The Ochkur approximation makes allowance for the effect of electron-exchange ignored in Born's approximation, and hence is capable of providing spin change cross sections (which are brought about solely by electron exchange).

The highly accurate 55 parameter helium wavefunctions of Weiss were used by Kim and Inokuti to provide highly accurate Form-factors (4). With this

knowledge, very accurate cross sections for (1) can be obtained from (2) and (3). The oscillator strengths f_{12} , the energy differences E_{21} and the line-strengths S_{12} for the various optically allowed transitions investigated are given in Table I.

5. Results and Discussion

In figs. (1-3) are presented the Born excitation cross sections (in $\pi a_0^2 = 0.88 \cdot 10^{-16} \text{ cm}^2$) calculated to within 1% accuracy for the $2^{1,3}S - 2^{1,3}P$, $3^{1,3}S$, $3^{1,3}P$, $3^{1,3}D$ and $4^{1,3}P$ transitions in helium, as a function of incident electron speed v_i (a.u.) and energy E_i (eV). The linestrength S for the $2^{1,3}S - 2^{1,3}P$ transition is the largest and hence it is only to be expected that the collision cross section for this transition dominates. Fig. 2 demonstrates a remarkable feature. At low impact energies the cross sections are in the following descending order $3^{1D} > 3^{1S} > 3^{1P} > 4^{1P}$, while at the high impact energies the natural order $3^{1P} > 3^{1D} > 3^{1S} > 4^{1P}$ is followed. For the singlet transitions, $\sigma(3^{1S}) > \sigma(3^{1P})$ from threshold to ~ 10 eV, while $\sigma(3^{1D}) > \sigma(3^{1P})$ to ~ 100 eV. Fig. 3 shows the corresponding behavior for the triplet transitions: at low energies $3^{3D} > 3^{3S} > 3^{3P} > 4^{3P}$ while for energies > 1000 eV (not shown in the fig. but see tables) the natural order is followed. Note $\sigma(3^{3S}) > \sigma(3^{3P})$ up to energies ~ 100 eV.

I believe that the reason for this very real behavior is that the line-strength for the $2^{1,3}S - 3^{1,3}P$ transition in helium is abnormally small ~ 2.5 to be compared with the value 18.8 for the $2s - 3p$ transition atomic hydrogen. It is also for this reason that I suggest that both $\sigma(4^{1D})$ and $\sigma(4^{1S})$ may well be of the same order of magnitude as $\sigma(3^{1P})$. At present we are seeking highly accurate wavefunctions in order to test this suggestion.

In the Born approximation, only the direct coupling between the initial and final state is taken into account. It may be possible that a theory taking account of virtual couplings will enhance the $2^1S - 3^1P$ transition via the $3^1S - 3^1P$ and $3^1D - 3^1P$ dipole couplings, at the expense of $\sigma(3^1D)$ and $\sigma(3^1S)$. This observation is worth investigation.

We expect the Born approximation for excitation from the helium metastables to the $n = 3$ and $n = 4$ levels to be valid down to rather low incident speeds (2-3 times threshold) because the excitation energies are rather small (see page 6). On the other hand, we do not expect the approximation to be valid at these low incident speeds for a "strong-coupling" case (large linestrength S) as with the $2^1S - 2^1P$ transition in helium (e.g. $S(2^1S - 2^1P) = 25$, $S(2^1S - 3^1P) = 2.5$, $S(2^1S - 3^1S,D) = 0$). However, even in this extreme case of strong coupling comparison with the elaborate close coupling calculations of Burke et al. (who have done only the $2^{1,3}S - 2^{1,3}P$ transitions) shows remarkable agreement with the Born results for energies ≥ 13 eV. If Born's approximation yields this agreement for the extreme $2^1S - 2^1P$ case, then for the weaker coupling $2^{1,3}S - 3^{1,3}L$ the validity is expected to be even better.

In Tables II-XI are tabulated the Born cross sections and the Ochkur cross sections. It is observed that the effect of electron exchange is apparently most marked for energies near threshold and decreases with increase of impact energy until it essentially disappears.

The Born cross sections are extremely valuable in that (a) they have been computed using highly accurate 55-parameter wavefunctions, (b) they can be used as a theoretical "yardstick", and (c) their comparison with experimental data would provide extremely direct and useful information on the general validity of Born's approximation for excited states.

6. Current Research

Methods applicable to ionization of metastables are being evaluated and again, since there are no calculations available except a Gryzinski-type classical application, pilot calculations on several theories are being carried out.

For excitation, the quantal and semiclassical close coupling methods and the attractive VPS methods are being currently explored.

7. Personnel Involved in the Research

1. M. R. Flannery - Principal Investigator
2. D. T. That - Postdoctoral Fellow (beginning 1 January 1974) - Ph.D. Yale University (1973). Thesis Topic: Electron impact on He, H^- and O_2 near resonances.
3. K. J. McCann - Third-year Graduate Student.
4. B. Richmond - Second-year Graduate Student.

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1. P. G. Burke and A. J. Taylor, Proc. Phys. Soc. 92, 336 (1967).
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5. V. I. Ochkur, Soviet Physics - JETP, 18, 503 (1964).
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10. A. J. Dixon (1973, private communication: Culham Laboratory, England).

Table 1: Oscillator Strengths f_{12} and line strengths S_{12} for helium
transitions.

1: initial state 2: final state

Initial state

Final state	2 $1P$	3 $1P$	4 $1P$	2 $3P$	3 $3P$	4 $3P$
Excitation energy (eV)	0.602	2.471	3.126	1.144	3.187	3.922
f_{12}	0.3764	0.1514	0.0507	0.5391	0.0645	0.0231
S_{12}	25.50	2.5	0.662	57.66	2.476	0.727

CASE 2-1/S TO 2-1/P E + HE(1S,2-1/S) = E + HE(1S,2-1/P) EN = .22131+01 A.U. = .60220+00 EV ERR = .010

		G(CM**2)		G(A0**2)		G(PI A0**2)	
E(EV)	V(A.U.)	BORN	CCHKUR	BORN	CCHKUR	BORN	CCHKUR
.40500+00	.21097+00	.12629-13	.32008-14	.45102+03	.11431+03	.14356+03	.36386+03
.62500+00	.21433+00	.34529-13	.95698-14	.12331+04	.34176+03	.39251+03	.10876+03
.65000+00	.21858+00	.47483-13	.14469-13	.16957+04	.51673+03	.53976+03	.16448+03
.70000+00	.22643+00	.61616-13	.21814-13	.22004+04	.77904+03	.70042+03	.24798+03
.75000+00	.23479+00	.69194-13	.27407-13	.24711+04	.97877+03	.78658+03	.31155+03
.10000+01	.27111+00	.77619-13	.42372-13	.27719+04	.15132+04	.88233+03	.48166+03
.25000+01	.42866+00	.51036-13	.42187-13	.18226+04	.15066+04	.58016+03	.47956+03
.40000+01	.54222+00	.37124-13	.33337-13	.13258+04	.11905+04	.42261+03	.37896+03
.45000+01	.57511+00	.34139-13	.31098-13	.12192+04	.11106+04	.38807+03	.35351+03
.50000+01	.60622+00	.31638-13	.29143-13	.11298+04	.10408+04	.35964+03	.33129+03
.60000+01	.66408+00	.27677-13	.25912-13	.98841+03	.92539+03	.31462+03	.29456+03
.80000+01	.76681+00	.22258-13	.21243-13	.79489+03	.75863+03	.25302+03	.24146+03
.10000+02	.85732+00	.18743-13	.18064-13	.66935+03	.64583+03	.21306+03	.20557+03
.15000+02	.10500+01	.13623-13	.13325-13	.48651+03	.47587+03	.15486+03	.15147+03
.20000+02	.12124+01	.10815-13	.10646-13	.38623+03	.38020+03	.12294+03	.12102+03
.30000+02	.14849+01	.77606-14	.76848-14	.27715+03	.27444+03	.88218+02	.87357+02
.40000+02	.17146+01	.61159-14	.60731-14	.21841+03	.21688+03	.69523+02	.69036+02
.50000+02	.19170+01	.50760-14	.50486-14	.18128+03	.18029+03	.57702+02	.57390+02
.70000+02	.22683+01	.38233-14	.38092-14	.13654+03	.13603+03	.43461+02	.43301+02
.10000+03	.27111+01	.28232-14	.28163-14	.10082+03	.10058+03	.32093+02	.32015+02

CASE 2-1/S TO 2-1/P

CASE 2-1/8 TO 3-1/8 E + HE(1S,2-1/8) = E + HE(1S,3-1/8) EN = .84716-01 A.L. = .23052+01 EV ERR = .010

		Q(CM**2)		Q(A0**2)		Q(FI A0**2)	
E(EV)	V(A.U.)	BORN	CCFKUR	BORN	CCFKUR	BORN	CCFKUR
.22150+01	.41250+00	.11267-15	.28836-16	.40236+01	.10298+01	.12608+01	.32780+00
.23250+01	.41339+00	.15907-15	.41662-16	.56808+01	.14878+01	.18082+01	.47360+00
.23500+01	.41560+00	.23555-15	.65117-16	.84121+01	.23254+01	.26777+01	.74021+00
.23750+01	.41781+00	.28972-15	.84141-16	.10346+02	.30048+01	.32934+01	.95647+00
.30000+01	.46958+00	.66425-15	.34694-15	.23722+02	.12390+02	.75509+01	.39439+01
.32500+01	.48875+00	.69461-15	.40112-15	.24806+02	.14325+02	.76960+01	.45596+01
.35000+01	.50720+00	.70624-15	.43836-15	.25221+02	.15655+02	.80282+01	.49531+01
.40000+01	.54222+00	.69977-15	.47917-15	.24990+02	.17112+02	.79546+01	.54470+01
.45000+01	.57511+00	.67574-15	.49327-15	.24132+02	.17616+02	.76814+01	.56072+01
.50000+01	.60622+00	.64550-15	.49301-15	.23052+02	.17606+02	.73377+01	.56043+01
.60000+01	.66408+00	.58334-15	.47303-15	.20832+02	.16893+02	.66312+01	.53772+01
.80000+01	.76691+00	.47825-15	.41335-15	.17079+02	.14762+02	.54365+01	.46987+01
.10000+02	.85732+00	.40124-15	.35899-15	.14329+02	.12820+02	.45611+01	.40808+01
.15000+02	.10590+01	.28319-15	.26397-15	.10113+02	.94269+01	.32192+01	.30007+01
.20000+02	.12124+01	.21845-15	.20752-15	.76013+01	.74110+01	.24832+01	.23590+01
.30000+02	.14849+01	.14967-15	.14477-15	.53450+01	.51699+01	.17014+01	.16455+01
.40000+02	.17146+01	.11372-15	.11095-15	.40611+01	.39621+01	.12927+01	.12612+01
.50000+02	.19170+01	.91310-16	.89531-16	.32609+01	.31973+01	.10360+01	.10177+01
.70000+02	.22683+01	.65804-16	.64894-16	.23500+01	.23175+01	.74203+00	.73768+00
.10000+03	.27111+01	.46374-16	.45927-16	.16501+01	.16401+01	.52715+00	.52207+00

CASE 2-1/8 TO 3-1/8

Table III

CASE 2-1/S TO 3-1/P E + HE(1S,2-1/S) = E + HE(1S,3-1/F) EN = .90640-01 A.L. = .24718+01 EV ERR = .010

G(CM**2)

G(A0**2)

G(PI A0**2)

E(EV)	V(A.U.)	BORN	CCPKUR	BORN	CCPKUR	BORN	CCPKUR
.24750+01	.42651+00	.18781-16	.46731-17	.67072+00	.16689+00	.21350+00	.53121-01
.25000+01	.42866+00	.54635-16	.13125-16	.19511+01	.46872+00	.62106+00	.14920+00
.27500+01	.44958+00	.13677-15	.26220-16	.48842+01	.93636+00	.15547+01	.29605-00
.30000+01	.46958+00	.15794-15	.30741-16	.56405+01	.10978+01	.17954+01	.34945-00
.32500+01	.48875+00	.16766-15	.38555-16	.59874+01	.13769+01	.19058+01	.43827+00
.35000+01	.50720+00	.17468-15	.49420-16	.62382+01	.17649+01	.19657+01	.56178+00
.37500+01	.52500+00	.18117-15	.62194-16	.64699+01	.22211+01	.20594+01	.70695+00
.40000+01	.54222+00	.18770-15	.75812-16	.67030+01	.27074+01	.21330+01	.86120+00
.45000+01	.57511+00	.20107-15	.10309-15	.71807+01	.36817+01	.22857+01	.11719+01
.50000+01	.60622+00	.21378-15	.12816-15	.76344+01	.45768+01	.24301+01	.14560+01
.60000+01	.66408+00	.23539-15	.16910-15	.84064+01	.60391+01	.26750+01	.19223+01
.80000+01	.76681+00	.25992-15	.21725-15	.92823+01	.77583+01	.29540+01	.24896+01
.10000+02	.85732+00	.26766-15	.23843-15	.95588+01	.85148+01	.30427+01	.27102+01
.15000+02	.10500+01	.26003-15	.24574-15	.92860+01	.87759+01	.29556+01	.27935+01
.20000+02	.12124+01	.24223-15	.23382-15	.86505+01	.83501+01	.27535+01	.26574+01
.30000+02	.14849+01	.20836-15	.20445-15	.74408+01	.73013+01	.23685+01	.23241+01
.40000+02	.17146+01	.18213-15	.17989-15	.65043+01	.64241+01	.20704+01	.20047+01
.50000+02	.19170+01	.16210-15	.16065-15	.57890+01	.57370+01	.18427+01	.18262+01
.70000+02	.22683+01	.13357-15	.13282-15	.47702+01	.47432+01	.15184+01	.15097+01
.10000+03	.27111+01	.10696-15	.10659-15	.38198+01	.38064+01	.12159+01	.12116+01

CASE 2-1/S TO 3-1/P

Table IV

CASE 2-1/8 TO 3-1/D E + HE(1S,2-1/8) = E + HE(1S,3-1/D) EN = .90354-01 A.U. = .24580+01 EV ERR = .010

		Q(CM**2)		Q(A0**2)		Q(PI A0**2)	
E(EV)	V(A.U.)	BORN	CCPKUR	BORN	CCPKUR	BORN	CCPKUR
.24600+01	.42522+00	.11808-15	.29600-16	.42168+01	.10571+01	.13422+01	.33648+00
.24750+01	.42651+00	.39960-15	.10307-15	.14271+02	.36809+01	.45424+01	.11717-01
.25000+01	.42866+00	.62487-15	.16853-15	.22315+02	.60185+01	.71032+01	.19158+01
.27500+01	.44958+00	.14287-14	.52911-15	.51023+02	.18895+02	.18241+02	.60145-01
.30000+01	.46958+00	.17075-14	.76201-15	.60977+02	.27213+02	.19410+02	.86621-01
.32500+01	.48875+00	.18306-14	.92613-15	.65374+02	.33074+02	.20809+02	.10528+02
.35000+01	.50720+00	.18803-14	.10420-14	.67150+02	.37213+02	.21374+02	.11845-02
.40000+01	.54222+00	.18789-14	.11764-14	.67099+02	.42013+02	.21355+02	.13373-02
.45000+01	.57511+00	.18180-14	.12323-14	.64925+02	.44008+02	.20666+02	.14008+02
.50000+01	.60622+00	.17370-14	.12451-14	.62031+02	.44465+02	.19745+02	.14154+02
.60000+01	.66408+00	.15682-14	.12103-14	.56004+02	.43221+02	.17627+02	.13758+02
.80000+01	.76581+00	.12633-14	.10720-14	.45828+02	.38282+02	.14548+02	.12186+02
.10000+02	.85732+00	.10759-14	.93725-15	.38422+02	.33471+02	.12230+02	.10654+02
.15000+02	.10500+01	.75931-15	.69589-15	.27117+02	.24852+02	.86315+01	.79105+01
.20000+02	.12124+01	.58501-15	.54885-15	.20892+02	.19601+02	.66501+01	.62391-01
.30000+02	.14849+01	.40023-15	.38396-15	.14293+02	.13712+02	.45497+01	.43647+01
.40000+02	.17146+01	.30394-15	.29474-15	.10854+02	.10526+02	.34551+01	.33504+01
.50000+02	.19170+01	.24493-15	.23902-15	.87469+01	.85358+01	.27842+01	.27170+01
.70000+02	.22683+01	.17627-15	.17324-15	.62951+01	.61869+01	.20038+01	.19693+01
.10000+03	.27111+01	.12416-15	.12267-15	.44338+01	.43807+01	.14113+01	.13944+01
CASE 2-1/8 TO 3-1/D							

Table V

CASE 2-1/S TO 4-1/P E + HE(1S,2-1/S) = E + HE(1S,4-1/P) EA = .11502+00 A.U. = .31297+01 EV ERR = .010

		Q(CM**2)		Q(A0**2)		Q(PI A0**2)	
E(EV)	V(A.U.)	BORN	CCPKUR	BORN	CCPKUR	BORN	CCPKUR
.31300+01	.47964+00	.95520-18	.23871-18	.34112-01	.85247-02	.10858-01	.27135-02
.31500+01	.48117+00	.84291-17	.20451-17	.30102+00	.73034-01	.95616-01	.23247-01
.32000+01	.48498+00	.15072-16	.34175-17	.53824+00	.12204+00	.17133+00	.36848-01
.32500+01	.48875+00	.18937-16	.40392-17	.67628+00	.14425+00	.21527+00	.45915-01
.33500+01	.49621+00	.23825-16	.46364-17	.85083+00	.16558+00	.27063+00	.52704-01
.35000+01	.50720+00	.28065-16	.51403-17	.10023+01	.18357+00	.31903+00	.59433-01
.37500+01	.52500+00	.31955-16	.62985-17	.11412+01	.22493+00	.36325+00	.71599-01
.40000+01	.54222+00	.34464-16	.81956-17	.12308+01	.29268+00	.39177+00	.93164-01
.45000+01	.57511+00	.38692-16	.13579-16	.13818+01	.48492+00	.43983+00	.15435+00
.50000+01	.60622+00	.42746-16	.19798-16	.15265+01	.70702+00	.48591+00	.22505+00
.60000+01	.66408+00	.50204-16	.31511-16	.17929+01	.11253+01	.57069+00	.35820+00
.80000+01	.76681+00	.60163-16	.47562-16	.21486+01	.16985+01	.68391+00	.54000+00
.10000+02	.85732+00	.64751-16	.55826-16	.23124+01	.19937+01	.73606+00	.63461+00
.15000+02	.10500+01	.65864-16	.61368-16	.23521+01	.21916+01	.74870+00	.69760+00
.20000+02	.12124+01	.62469-16	.59787-16	.22309+01	.21351+01	.71012+00	.67962+00
.30000+02	.14849+01	.54587-16	.53326-16	.19494+01	.19044+01	.62052+00	.60618+00
.40000+02	.17146+01	.48055-16	.47326-16	.17161+01	.16901+01	.54626+00	.53797+00
.50000+02	.19170+01	.42934-16	.42460-16	.15333+01	.15163+01	.48806+00	.48266+00
.70000+02	.22683+01	.35572-16	.35325-16	.12703+01	.12615+01	.40436+00	.40156+00
.10000+03	.27111+01	.28590-16	.28468-16	.10210+01	.10166+01	.32500+00	.32361+00

----- CASE 2-1/S TO 4-1/P

Table VI

CASE 2-3/S TO 2-3/P

 $E + HE(1S, 2-3/S) = E + HE(1S, 2-3/P)$ $EN = .42066-01 \text{ A.U.} = .11446+01 \text{ EV}$

ERR = .010

Q(CP**2)

Q(A0**2)

Q(PI A0**2)

E(EV)

V(A.U.)

BORN

CCHKUR

BORN

CCHKUR

BCPA

CCHKUR

.11500+01	.29073+00	.42410-14	.31902-14	.15146+03	.11393+03	.48210+02	.30265+02
.12500+01	.30311+00	.16862-13	.13258-13	.60218+03	.47348+03	.19160+03	.15071+03
.15000+01	.33204+00	.24404-13	.20275-13	.87150+03	.72406+03	.27741+03	.23042+03
.17500+01	.35864+00	.26094-13	.22149-13	.93188+03	.79099+03	.29063+03	.25170+03
.20000+01	.38341+00	.26103-13	.22357-13	.93218+03	.79842+03	.29572+03	.25415+03
.30000+01	.46958+00	.22946-13	.20002-13	.81945+03	.71430+03	.26064+03	.22737+03
.35000+01	.50720+00	.21260-13	.18701-13	.75924+03	.66785+03	.24167+03	.21257+03
.40000+01	.54222+00	.19783-13	.17567-13	.70649+03	.62735+03	.22485+03	.19969+03
.45000+01	.57511+00	.18492-13	.16570-13	.66037+03	.59176+03	.21020+03	.18836+03
.50000+01	.60622+00	.17362-13	.15691-13	.62004+03	.56034+03	.19735+03	.17836+03
.60000+01	.66408+00	.15476-13	.14190-13	.55268+03	.50675+03	.17592+03	.16130+03
.80000+01	.76681+00	.12787-13	.11974-13	.45666+03	.42761+03	.14536+03	.13611+03
.10000+02	.85732+00	.10951-13	.10395-13	.39108+03	.37124+03	.12448+03	.11817+03
.15000+02	.10500+01	.81635-14	.78961-14	.29154+03	.28199+03	.92799+02	.89759+02
.20000+02	.12124+01	.65784-14	.64222-14	.23493+03	.22935+03	.74779+02	.73004+02
.30000+02	.14849+01	.48030-14	.47310-14	.17152+03	.16895+03	.54592+02	.53760+02
.40000+02	.17146+01	.38261-14	.37849-14	.13664+03	.13517+03	.43494+02	.43025+02
.50000+02	.19170+01	.31996-14	.31730-14	.11427+03	.11331+03	.36372+02	.36069+02
.70000+02	.22693+01	.24349-14	.24211-14	.86954+02	.86463+02	.27678+02	.27522+02
.10000+03	.27111+01	.18155-14	.18087-14	.64836+02	.64594+02	.20638+02	.20561+02

CASE 2-3/S TO 2-3/P

Table VII

CASE 2-3/S TO 3-3/S E + HE(1S,2-3/S) = E + HE(1S,3-3/S) FN = .10654+00 A.L. = .28991+01 EV ERR = .010

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		Q(CM**2)		Q(A0**2)		Q(PI A0**2)	
E(EV)	V(A.L.)	BORN	CCHKUR	BORN	CCHKUR	BORN	CCHKUR
.29000+01	.46168+00	.19046-16	.14285-16	.68018+00	.51014+00	.21651+00	.16238+00
.30000+01	.46958+00	.18959-15	.14234-15	.67708+01	.50833+01	.21552+01	.16181+01
.32500+01	.48875+00	.31334-15	.23506-15	.11190+02	.83946+01	.35619+01	.26721+01
.35000+01	.50720+00	.36755-15	.27525-15	.13126+02	.98299+01	.41782+01	.31290+01
.37500+01	.52500+00	.39557-15	.29743-15	.14127+02	.10622+02	.44967+01	.33811+01
.40000+01	.54222+00	.40987-15	.30955-15	.14637+02	.11055+02	.46592+01	.35188+01
.42500+01	.55291+00	.41611-15	.31645-15	.14860+02	.11301+02	.47301+01	.35972+01
.45000+01	.57511+00	.41741-15	.31977-15	.14906+02	.11420+02	.47449+01	.36350+01
.47500+01	.59087+00	.41530-15	.32085-15	.14831+02	.11458+02	.47209+01	.36473+01
.50000+01	.60622+00	.41107-15	.32039-15	.14680+02	.11442+02	.46729+01	.36420+01
.60000+01	.66488+00	.38418-15	.30979-15	.13720+02	.11063+02	.43672+01	.35216+01
.80000+01	.76681+00	.32453-15	.27539-15	.11590+02	.98347+01	.36891+01	.31305+01
.10000+02	.85732+00	.27623-15	.24215-15	.98646+01	.86478+01	.31400+01	.27527+01
.15000+02	.10570+01	.19831-15	.18170-15	.70820+01	.64687+01	.22543+01	.20654+01
.20000+02	.12124+01	.15385-15	.14411-15	.54942+01	.51464+01	.17489+01	.16381+01
.30000+02	.14849+01	.10594-15	.10144-15	.37834+01	.36227+01	.12043+01	.11531+01
.40000+02	.17146+01	.80711-16	.78132-16	.28823+01	.27903+01	.51748+00	.88816+00
.50000+02	.19170+01	.65166-16	.63497-16	.23272+01	.22676+01	.74077+00	.72181+00
.70000+02	.22683+01	.47026-16	.46164-16	.16794+01	.16486+01	.53456+00	.52477+00
.10000+03	.27111+01	.33170-16	.32744-16	.11846+01	.11694+01	.37706+00	.37222+00

===== CASE 2-3/S TO 3-3/S

Table VIII

CASE 2-3/S TO 3-3/P

E + HE(1S,2-3/S) = E + HE(1S,3-3/P)

EN = .11717+00 A.U. = .31882+01 EV

ERN = .010

Q(CM**2)

Q(A0**2)

Q(PI A0**2)

E(EV)	V(A.U.)	BORN	CCHKUR	FORN	CCHKUR	BLFN	CCHKUR
.32000+01	.48498+00	.30494-16	.23036-16	.10890+01	.62266+00	.34664+00	.26186+00
.32250+01	.48697+00	.52708-16	.40405-16	.18823+01	.14429+01	.59916+00	.45530+00
.32500+01	.48875+00	.66843-16	.51955-16	.23871+01	.18554+01	.75964+00	.59060+00
.35000+01	.50720+00	.12219-15	.10538-15	.43637+01	.37633+01	.13890+01	.11979+01
.37500+01	.52500+00	.13629-15	.12476-15	.46671+01	.44555+01	.15492+01	.14182+01
.40000+01	.54222+00	.13876-15	.13143-15	.49553+01	.46937+01	.15773+01	.14940+01
.42500+01	.55891+00	.13676-15	.12918-15	.48841+01	.46131+01	.15546+01	.14684+01
.45000+01	.57511+00	.13308-15	.12505-15	.47527+01	.44659+01	.15126+01	.14215+01
.47500+01	.59087+00	.12890-15	.11956-15	.46032+01	.42699+01	.14653+01	.13591+01
.50000+01	.60622+00	.12476-15	.11374-15	.44553+01	.40617+01	.14182+01	.12929+01
.60000+01	.66408+00	.11152-15	.94417-16	.39826+01	.33718+01	.12677+01	.10733+01
.80000+01	.76681+00	.98034-16	.78219-16	.35010+01	.27934+01	.11144+01	.88916+00
.10000+02	.85732+00	.91547-16	.74285-16	.32693+01	.26529+01	.10407+01	.84444+00
.15000+02	.10500+01	.81986-16	.71520-16	.29279+01	.25541+01	.93192+00	.81301+00
.20000+02	.12124+01	.74832-16	.68143-16	.26724+01	.24335+01	.85065+00	.77461+00
.30000+02	.14849+01	.63957-16	.60623-16	.22840+01	.21650+01	.72703+00	.68913+00
.40000+02	.17146+01	.56031-16	.54053-16	.20010+01	.19304+01	.63693+00	.61445+00
.50000+02	.19170+01	.50018-16	.48713-16	.17863+01	.17396+01	.56658+00	.55375+00
.70000+02	.22693+01	.41495-16	.40806-16	.14819+01	.14573+01	.47169+00	.46386+00
.10000+03	.27111+01	.33454-16	.33107-16	.11947+01	.11823+01	.38028+00	.37635+00

CASE 2-3/S TO 3-3/P

Table IX

CASE 2-3/S TO 3-3/D E + HE(1S,2-3/S) = E + HE(1S,3-3/D) EN = .11959+00 A.U. = .32542+01 EV ERR = .010

		G(CM**2)		G(A0**2)		G(PI A0**2)	
E (EV)	V(A.U.)	BORN	CCPKUR	BORN	CCPKUR	BORN	CCPKUR

.33000+01	.49250+00	.20847-15	.15644-15	.74448+01	.55866+01	.23692+01	.17783+01
.33250+01	.49436+00	.25651-15	.19254-15	.91605+01	.68759+01	.26159+01	.21887+01
.33500+01	.49621+00	.29530-15	.22170-15	.10546+02	.79175+01	.33565+01	.25292+01
.35000+01	.50720+00	.44522-15	.33465-15	.15900+02	.11951+02	.50611+01	.37042+01
.37500+01	.52500+00	.57535-15	.43275-15	.20547+02	.15454+02	.65403+01	.49192+01
.40000+01	.54222+00	.64570-15	.48627-15	.23059+02	.17366+02	.73400+01	.55277+01
.42500+01	.55891+00	.68633-15	.51774-15	.24510+02	.18489+02	.78619+01	.58854+01
.45000+01	.57511+00	.70939-15	.54076-15	.25334+02	.19312+02	.80640+01	.61471+01
.47500+01	.59087+00	.72125-15	.55366-15	.25757+02	.19772+02	.81960+01	.62937+01
.50000+01	.60622+00	.72607-15	.56093-15	.25929+02	.20032+02	.82535+01	.63764+01
.60000+01	.66408+00	.70552-15	.56119-15	.25196+02	.20041+02	.80200+01	.63792+01
.80000+01	.76681+00	.61630-15	.51502-15	.22009+02	.18393+02	.70057+01	.56845+01
.10000+02	.85732+00	.53261-15	.46054-15	.19021+02	.16447+02	.60544+01	.52352+01
.15000+02	.10500+01	.38895-15	.35289-15	.13890+02	.12602+02	.44214+01	.40114+01
.20000+02	.12124+01	.30394-15	.28258-15	.10854+02	.10091+02	.34551+01	.32122+01
.30000+02	.14849+01	.21069-15	.20073-15	.75242+01	.71685+01	.23950+01	.22614+01
.40000+02	.17146+01	.16102-15	.15529-15	.57503+01	.55456+01	.18304+01	.17652+01
.50000+02	.19170+01	.13025-15	.12653-15	.46514+01	.45187+01	.14806+01	.14383+01
.70000+02	.22683+01	.94191-16	.92267-16	.33638+01	.32950+01	.10767+01	.10488+01
.10000+03	.27111+01	.66534-16	.65581-16	.23761+01	.23420+01	.75632+00	.74544+01

CASE 2-3/S TO 3-3/D

Table X

CASE 2-3/S TO 4-3/P E + HE(1S,2-3/9) = E + HE(1S,4-3/P) EN = .14303+00 A.U. = .38921+01 EV EPR = .010

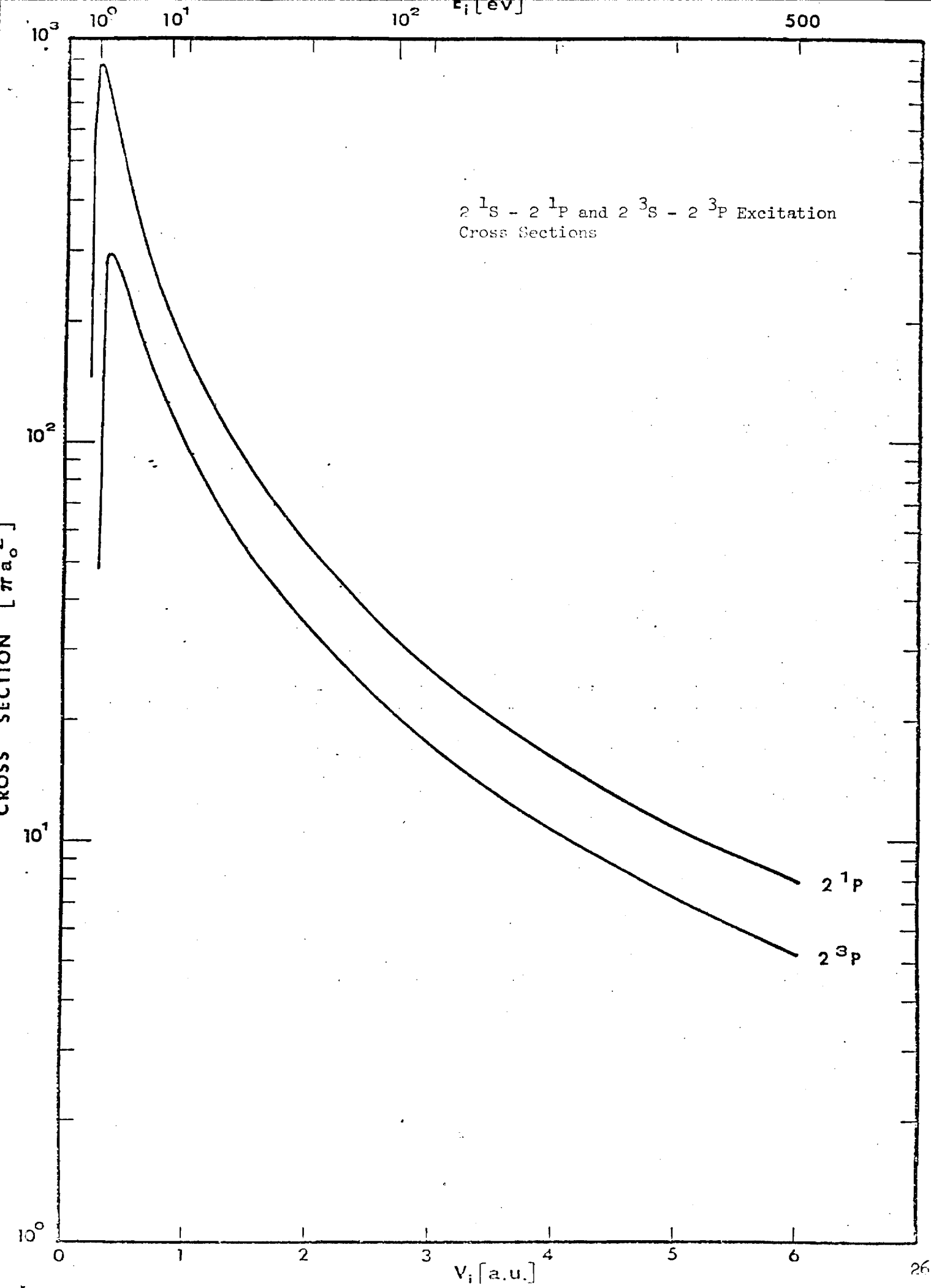
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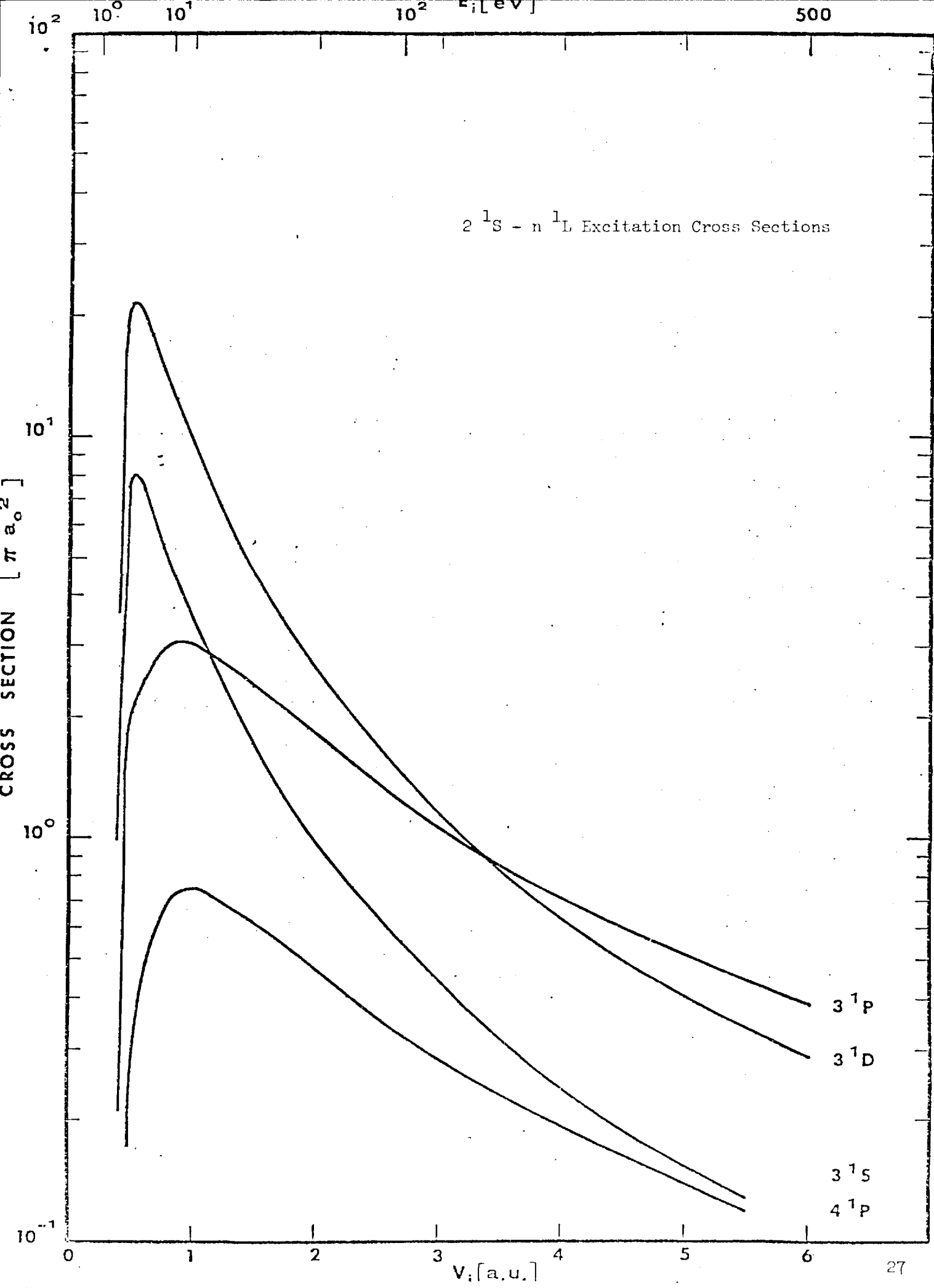
		Q(CM**2)		Q(A0**2)		Q(PI A0**2)	
E(EV)	V(A.U.)	BORN	CHKUR	PCRN	CHKUR	PCRN	CHKUR
.38950+01	.53506+00	.30590-17	.22982-17	.10924+00	.82073-01	.34773-01	.26125-01
.39000+01	.53540+00	.50053-17	.37713-17	.17875+00	.13468+00	.56698-01	.42470-01
.39250+01	.53711+00	.99947-17	.76365-17	.35693+00	.27271+00	.11361+00	.86908-01
.39500+01	.53822+00	.13002-16	.10067-16	.46434+00	.35952+00	.14781+00	.11444+00
.39750+01	.54052+00	.15265-16	.11969-16	.54516+00	.42744+00	.17353+00	.13606+00
.40000+01	.54222+00	.17091-16	.13562-16	.61035+00	.48434+00	.19426+00	.15417+00
.42500+01	.55891+00	.26001-16	.22646-16	.92856+00	.60875+00	.29557+00	.25741+00
.45000+01	.57511+00	.28845-16	.26468-16	.10301+01	.94523+00	.32790+00	.30068+00
.47500+01	.59067+00	.29659-16	.27951-16	.10592+01	.99817+00	.33710+00	.31773+00
.50000+01	.60622+00	.29630-16	.28168-16	.10582+01	.10059+01	.33682+00	.32020+00
.60000+01	.66408+00	.27672-16	.25058-16	.98621+00	.89486+00	.31456+00	.26484+00
.80000+01	.76681+00	.25290-16	.20565-16	.90317+00	.73442+00	.26749+00	.23377+00
.10000+02	.85732+00	.24466-16	.19746-16	.87372+00	.70518+00	.27811+00	.22447+00
.15000+02	.10500+01	.23131-16	.19973-16	.82604+00	.71329+00	.26294+00	.22705+00
.20000+02	.12124+01	.21670-16	.19590-16	.77388+00	.69958+00	.24633+00	.22268+00
.30000+02	.14849+01	.18948-16	.17886-16	.67668+00	.63875+00	.21539+00	.20332+00
.40000+02	.17146+01	.16742-16	.16106-16	.59790+00	.57518+00	.19032+00	.18306+00
.50000+02	.19170+01	.15024-16	.14602-16	.53654+00	.52146+00	.17079+00	.16599+00
.70000+02	.22683+01	.12532-16	.12308-16	.44756+00	.43955+00	.14246+00	.13991+00
.10000+03	.27111+01	.10139-16	.10026-16	.36209+00	.35606+00	.11526+00	.11397+00

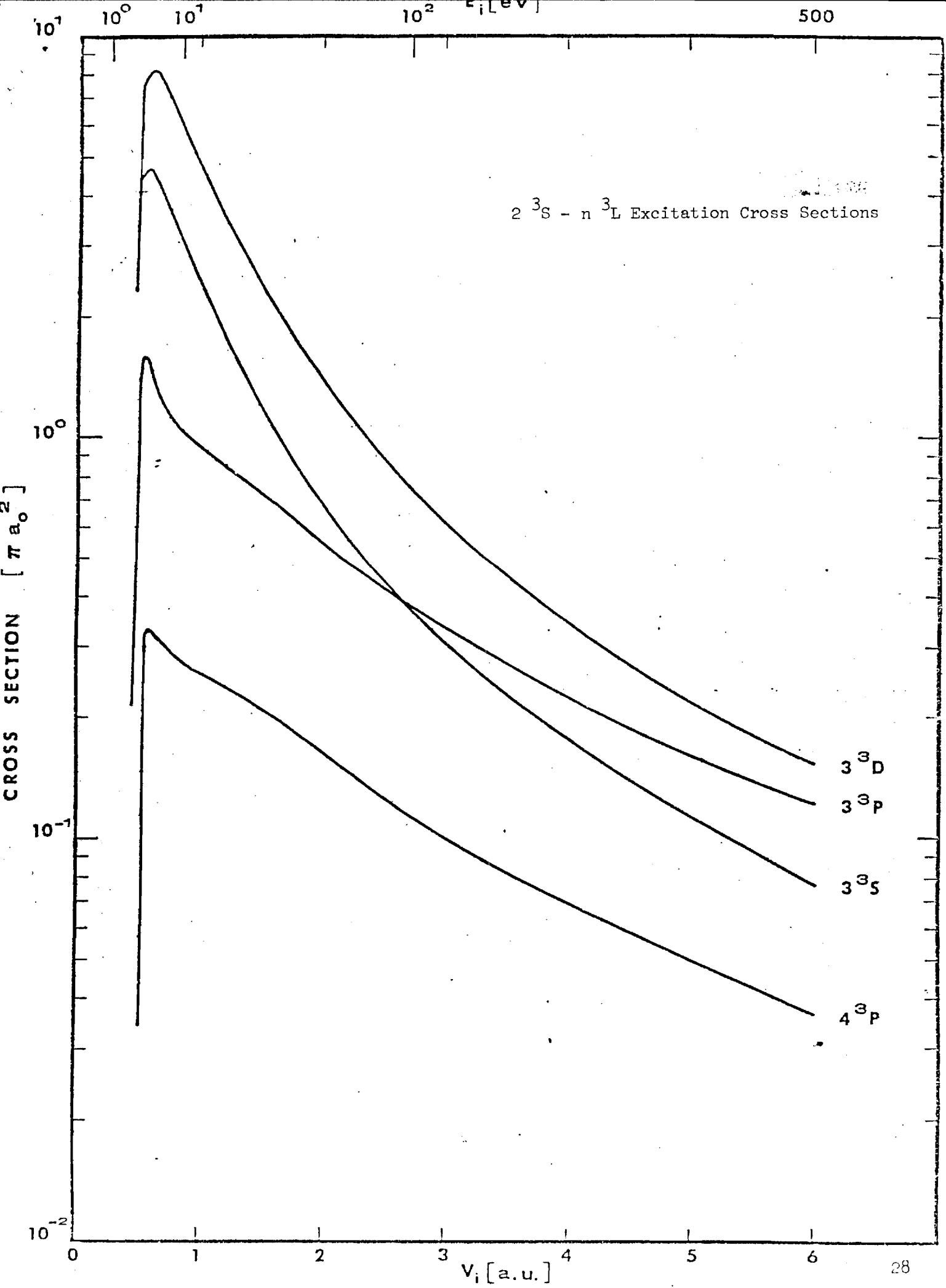
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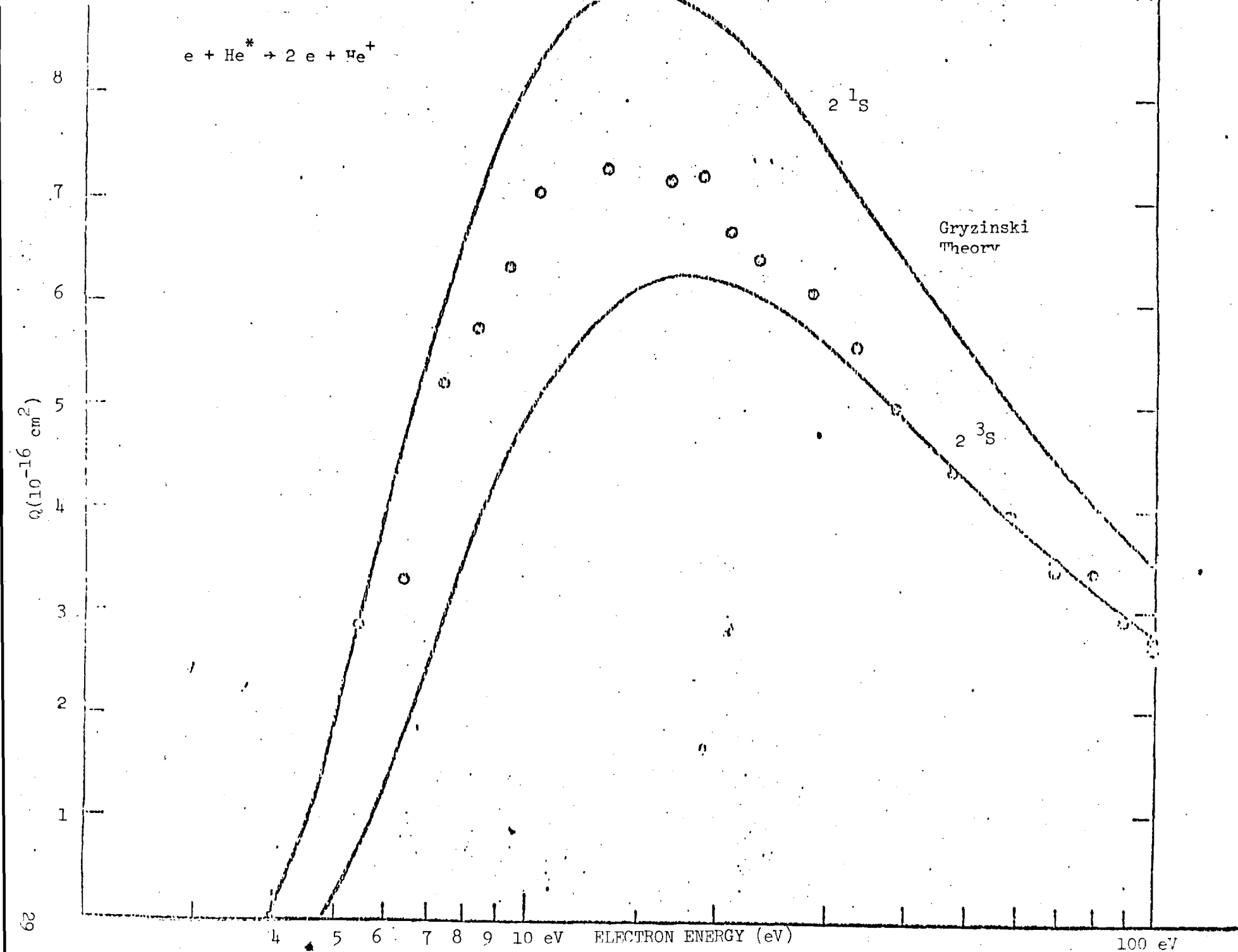
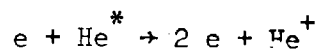
CASE 2-3/S TO 4-3/P

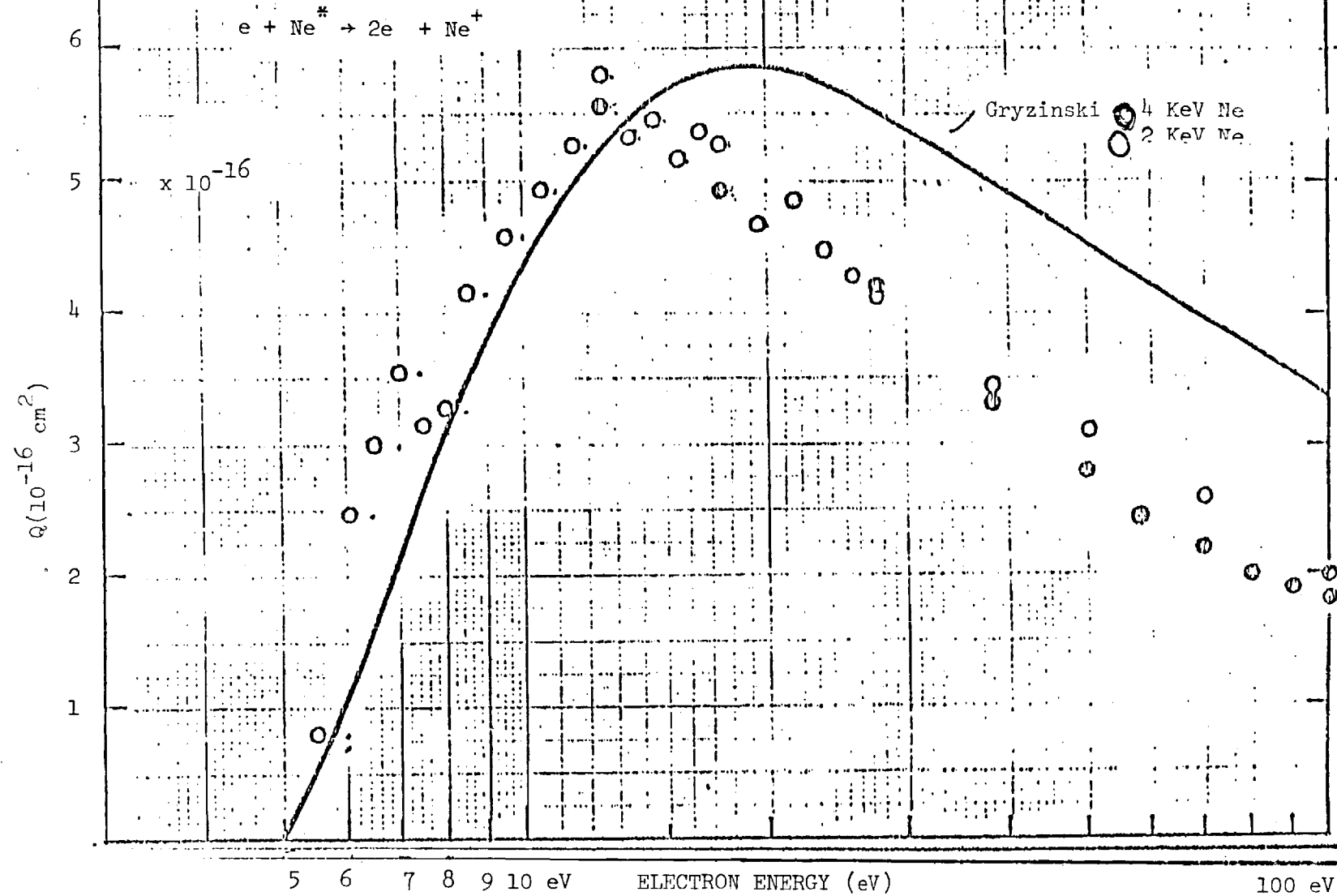
Table XI

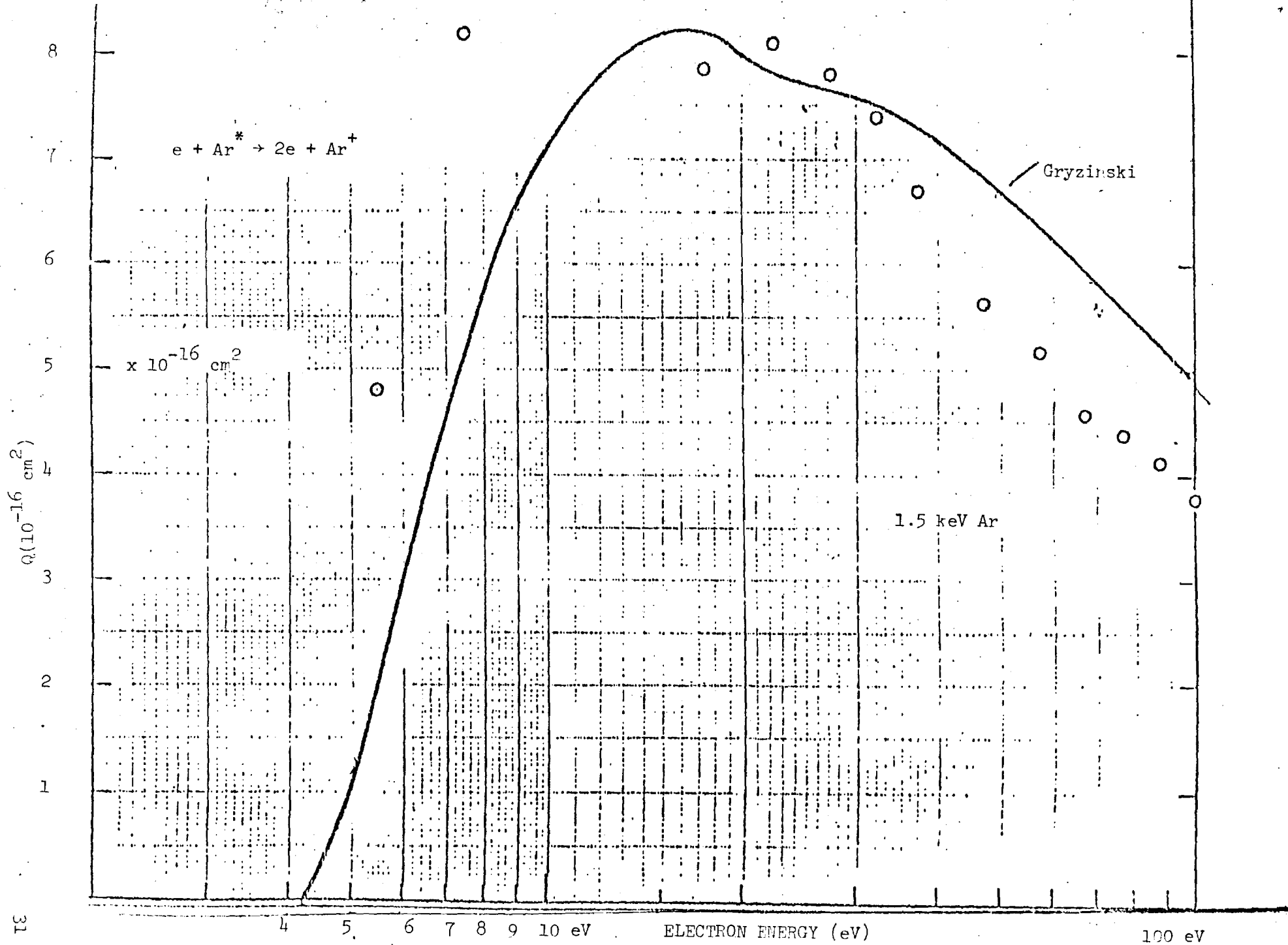












6-4f-631

GEORGIA INSTITUTE OF TECHNOLOGY
ATLANTA, GEORGIA 30332

July 9, 1974

SCHOOL OF PHYSICS

Air Force Aerospace Research Laboratories

ATTN: ARL/DC

Contract F33615-74-C-4003

Item No. 0002, Sequence No.

Wright-Patterson AFB, OH 45433

SUBJECT: Quarterly R and D Status Report
Principal Investigator, M. R. Flannery
covering the period 3 April - 8 July 74

Gentlemen:

Transmitted herewith are four (4) copies of the subject report.

Should you have any questions or comments regarding this report,
please contact the principal investigator.

Sincerely,

M. R. Flannery

M. R. Flannery
Professor

MRF:rh

Enclosures

REPORT:

Second Quarterly R&D Status Report
covering the period April 8, 1974 - July 8, 1974

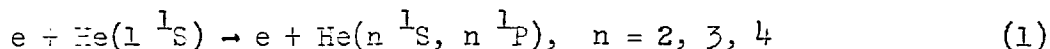
PROJECT-TITLE: Calculation of Electron Impact Cross Sections
from Metastable States in Atomic and Molecular Gases

PRINCIPAL INVESTIGATOR: M. R. Flannery
School of Physics
Georgia Institute of Technology
Atlanta, Georgia 30332

CONTRACT NO: F33615-74-C-4003

SPONSOR CONTACT PERSON: Lt. John F. Prince / Dr. Alan Garscadden
U.S. Air Force
Air Force Systems Command
Bldg. 450, Area B
Hg. 4950th Test Wing, 4950 (PM MA)
Wright-Patterson, AFB, Ohio 45433

Excitation: In an effort to probe its further usefulness and goodness, the Multichannel Eikonal Treatment of electron-atom collisions has been applied during this quarter to the examination of



The calculated cross sections are displayed in figs. (1-3) together with other theoretical results and experimental data. The overall agreement with experiment is impressive. Note that for the $n = 3$ and 4 excitations, the only other theoretical work is the Born approximation. The present treatment provides considerable improvement.

Ionization: The Vainshtein, Presnyakov and Sobelman approximation is currently being applied to the ionization of helium. Also, the ionization of neon is being examined in the Born Approximation. Careful theoretical consideration has to be given to the coupling scheme valid for the metastable states of Neon.

Publications: A paper entitled "The Multichannel Eikonal Treatment of Atomic Collisions: The $2\ ^1\text{S}$ and $2\ ^1\text{P}$ inelastic scattering of electrons by helium", was submitted for publication to Physical Review. The paper appears as Appendix A of this report

A paper of the above title has also been accepted for reading at the following two conferences.

- (1) "International Conference on Electron and photon interactions with atoms", at Stirling, Scotland
- (2) "The Fourth International Conference on Atomic Physics", at Heidelberg, Germany

and the abstract, in Appendix B, will appear in the respective books of abstracts.

In addition, the Committee of conference (1) has requested that I submit another paper so that it be included in a book. Festschrift in honor of Ugo Fano, Proceedings of conference (1) to be published by Plenum Press. The paper that I will be submitting is in Appendix C.

Our first article on the Eikonal Treatment has now appeared in J. Phys. B:
7 (1974) 1223.

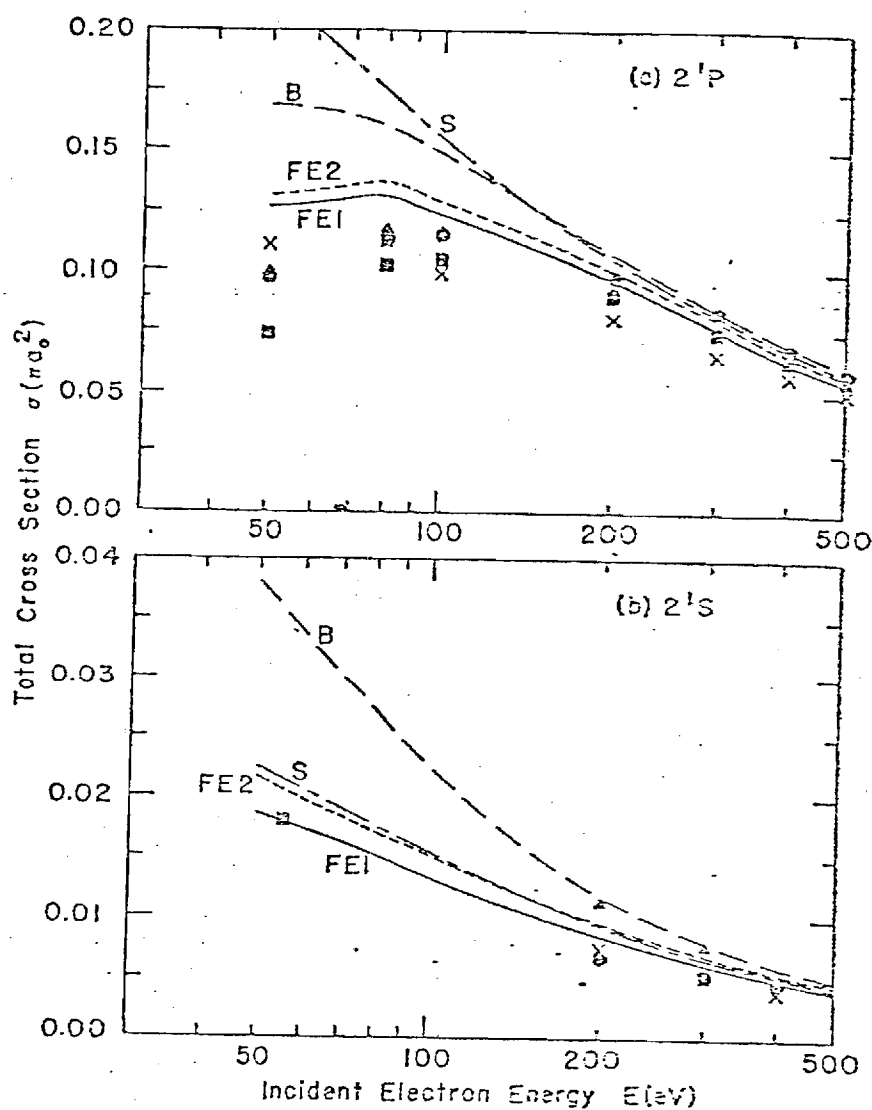


Figure 1: Total cross sections for (a) the 2^1P and (b) the 2^1S excitations of $\text{He}(1^1S)$ by electron impact. Theory: FE1: Four channel eikonal treatment with first set of atomic wavefunctions; FE2: Four channel eikonal treatment with set of atomic wavefunctions; S: Second-Order potential method with first set of atomic wavefunctions (Berrington et al. (1975)); B: Born-approximations (Bell et al. 1969). Experiment: (2^1P): A : Donaldson et al. (1972); B : Jobe and St. John (1967); X : Moustafa-Moussa (1969); O : van Eck and de Jongh (1970); (2^1S): A : Lassetire et al. (1970); X : Miller et al. (1963); O : Vriens et al. (1963).

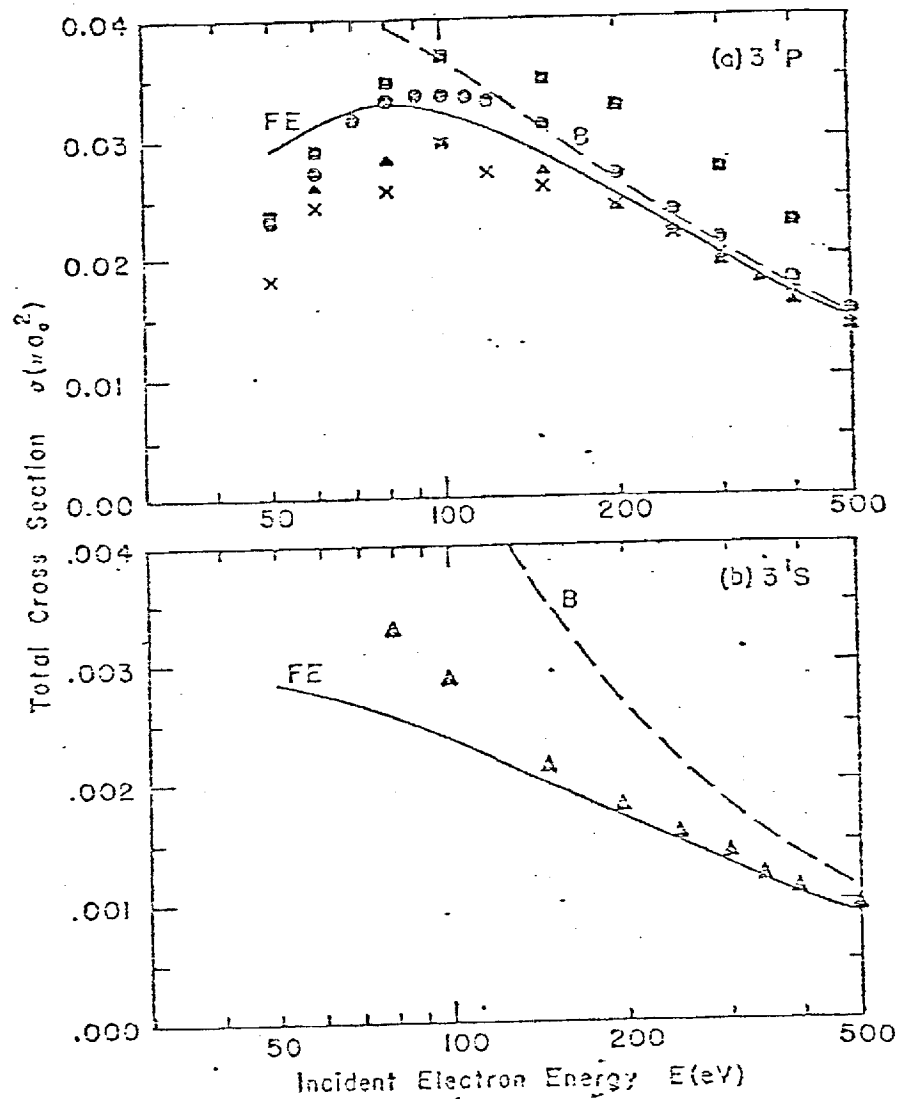


Figure 2: Total cross sections for (a) the 3^1P and (b) the 3^1S excitations of $\text{He}(1^1S)$ by electron impact. Theory: FE: Four channel eikonal treatment with Hartree-Fock frozen core wavefunctions; B: Born approximation (Bell et al. 1969). Experiment: \circ : Donaldson et al. (1972); \triangle : Moustafa Mousa et al. (1969); \times : van Eck and de Jongh (1970); \blacksquare : St. John et al. (1964).

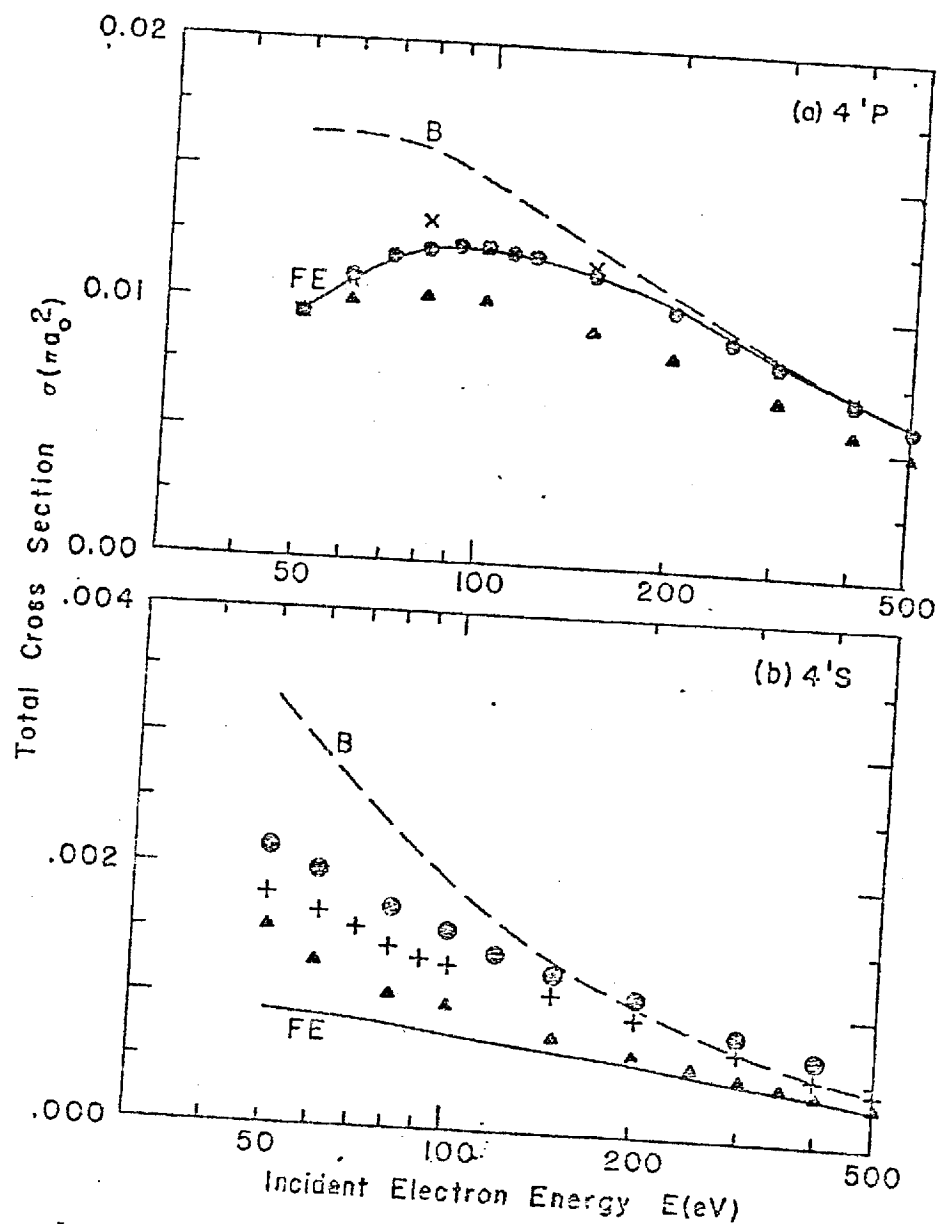


Figure 3: Total cross sections for (a) $4\ 1P$ and (b) the $3\ 1S$ excitations of $He(1\ 1S)$ by electron impact. FE: Present Four-Channel Eikonal; B: Born Approximation (Bell et al. 1969); \odot : Donaldson et al. 1972 ($4\ 1P$); McConkey et al. ($4\ 1S$), (1971); \blacktriangle : Moustafa-Musa et al. (1969); \times : de Jongh and van Eck (1971); $+$: van Raan et al. (1971).

APPENDIX A: The Multichannel Treatment of Atomic Collisions:
The 2^1S and 2^1P Inelastic Scattering of Electrons
by Helium.

(submitted to Phys. Rev.)

The Multichannel Eikonal Treatment of Atomic Collisions:
The 2^1S and 2^1P Inelastic Scattering of Electrons by Helium*

K. J. McCann and M. R. Flannery
School of Physics, Georgia Institute of Technology
Atlanta, Georgia 30332

A multichannel eikonal treatment of atomic collisions is presented and applied to the excitation of atomic helium by electrons with incident energy E in the range $50 \text{ eV} \leq E \leq 500 \text{ eV}$. Two different sets of orthogonal wavefunctions are employed. A four-channel description yields differential and total excitation cross sections in satisfactory agreement with experiment.

1. Introduction

Apart from the application of the first and second Born approximations¹⁻³, Ochkur modifications⁴, Glauber-type approaches^{5,6} and impact-parameter methods^{7,8} to collisional excitation of atomic helium by incident electrons, theoretical knowledge of these collisions for low and intermediate impact energies beyond the inelastic thresholds is very limited. The experimental measurement of the vacuum UV excitation functions is difficult⁹⁻¹⁹ and requires high resolution, and full account must be taken of cascade and other well-identified problems. In order to provide absolute cross sections, the measurements must then be normalized to some high-energy theoretical cross section, and the energy-point of departure of the actual cross sections from the corresponding Born or Bethe values is extremely uncertain.

In an effort to obtain an accurate description of electron-(excited) atom collisions in the intermediate energy region, a multistate-eikonal treatment of atomic collisions has recently been developed^{20,21}. The method achieved notable success for $e - H(1s)$ excitation and the resulting differential and total cross sections agreed closely with experiment and with other refined treatments. Moreover, the basic formulae which acknowledged different speeds in various channels reduced upon successive approximation to those obtained previously by other authors.^{5,22,23} In an effort to probe the further reliability of the present method, the 2^1S and the 2^1P excitations of atomic helium by electron impact are examined in this paper. The resulting total and differential cross sections are compared with previous treatments and with experiment.

Theory

The scattering amplitude describing a transition between an initial channel i and a final channel f of the electron-helium collision system of reduced mass μ is, in the center-of-mass reference frame,

$$f_{if}(\theta, \varphi) = -\frac{1}{4\pi} \frac{2u}{h} \langle \psi_f(\underline{k}_f; \underline{r}, R) | V(\underline{r}, R) | \psi_i^+(\underline{k}_i; \underline{r}, R) \rangle_{\underline{r}, R} \quad (1)$$

where $V(\underline{r}, R)$ is the instantaneous electrostatic interaction between the electron at \underline{r} and the helium atom with internal electronic coordinates denoted collectively by $\underline{r}_1, \underline{r}_2$, both vectors relative to the helium nucleus as origin. The wavenumbers of the relative motion in the initial and final channels asymptotically ($R \sim \infty$) tend to k_i and k_f respectively, the final stationary state of the isolated atom in channel f is ψ_f , and ψ_i^+ is the solution of the time independent Schrödinger equation,

$$\left[-\frac{\hbar^2}{2u} \nabla_R^2 + H_e(\underline{r}) + V(\underline{r}, R) \right] \psi_i^+(\underline{r}, R) = E_i \psi_i^+(\underline{r}, R) \quad (2)$$

solved subject to the asymptotic boundary condition.

$$\psi_i^+(\underline{r}, R) \xrightarrow{\text{large } R} \sum_n \left[e^{i \underline{k}_n \cdot \underline{R}} \delta_{ni} + f_{in}(\theta, \varphi) \frac{e^{i \underline{k}_n \cdot \underline{R}}}{R} \right] \phi_n(\underline{r}_1, \underline{r}_2) \quad (3)$$

in which $\phi_n(\underline{r}_1, \underline{r}_2)$ are eigenfunctions of the Hamiltonian $H_e(\underline{r})$ for the isolated helium atom with internal electronic energy \mathcal{E}_n such that the total energy E_i in channel i is $\mathcal{E}_i + \hbar^2 k_i^2 / 2u$ which is conserved throughout the collision. In the absence of the interaction the wavefunction for the system in the final channel is therefore $\phi_f(\underline{r}_1, \underline{r}_2) \exp(i \underline{k}_f \cdot \underline{R})$.

The Eikonal Approximation to (2) writes the total wavefunction in the presence of the interaction as

$$\psi_i^+(\underline{r}, R) = \sum_n A_n(\underline{r}, Z) \exp i S_n(\underline{r}, Z) \phi_n(\underline{r}_1, \underline{r}_2) \quad (4)$$

where the nuclear separation $\underline{R} \equiv (R, \Theta, \varphi) \equiv (\rho, \varphi, Z)$ in spherical and cylindrical coordinate frames respectively. The eikonal S_n in (4) is the characteristic-function solution of the classical Hamilton-Jacobi equation (i.e. the Schrodinger equation in the $\hbar \rightarrow 0$ limit) for the e - He relative motion under the static interaction $V_{nn}(\underline{R})$, and is therefore given by

$$S_n(\underline{R}, Z) = k_n Z + \int_{-\infty}^Z [K_n(\underline{R}) - k_n] dZ \quad (5)$$

in which the local wavenumber of relative motion at \underline{R} is

$$K_n(\underline{R}) = \left[k_n^2 - \frac{2u}{\hbar^2} V_{nn}(\underline{R}) \right]^{\frac{1}{2}}. \quad (6)$$

and where dZ is assumed to be an element of path length along the trajectory.

The interaction matrix elements coupling the various atomic states are

$$V_{nm}(\underline{R}) = \langle \varphi_n(\underline{r}_1, \underline{r}_2) | V(\underline{r}, \underline{R}) | \varphi_m(\underline{r}_1, \underline{r}_2) \rangle \quad (7)$$

By inserting (4) into (1) and with the aid of (2) - (7), Flannery and McCann²¹ have shown that the scattering amplitude then reduces to

$$f_{if}(\theta, \varphi) = -i^{\Delta+1} \int_0^\infty J_\Delta(K' \rho) [I_1(\rho, \theta) - i I_2(\rho, \theta)] \rho d\rho \quad (8)$$

where K' is the XY -component $k_F \sin \theta$ of \underline{K} and where J_Δ are Bessel functions of integral order. Both the functions

$$I_1(\rho, \theta; \alpha) = \int_{-\infty}^\infty K_F(\rho, Z) \left[\frac{\partial C_F(\rho, Z)}{\partial Z} \right] \exp(i\alpha Z) dZ \quad (9)$$

and

$$I_2(\rho, \theta; \alpha) = \int_{-\infty}^{\infty} \left[K_F(K_F - k_F) + \frac{\mu}{h} V_{FF} \right] C_F(\rho, Z) \exp(i\alpha Z) dZ \quad (10)$$

depend on the scattering angle θ via the parameter

$$\alpha = k_F(1 - \cos \theta) = 2k_F \sin^2 \frac{\theta}{2} \quad (11)$$

the difference between the Z-component of the momentum change \tilde{K} and the minimum momentum change $k_i - k_F$ in the collision. The transition amplitudes $C_F(\rho, Z)$ which are related to the original phase ϕ -dependent coefficients $A_F(\rho, Z)$ by,

$$C_F(\rho, Z) = A_F(\rho, Z) \exp \left(i \int_{-\infty}^Z (K_F - k_F) dZ \right) \exp(-i\Delta\phi) \quad (12)$$

where Δ is the change $M_i - M_F$ in the azimuthal quantum number of the atom, can be shown to satisfy the following set of N-coupled differential equations

$$\frac{i\hbar^2}{\mu} K_F(\rho, Z) \frac{\partial C_F(\rho, Z)}{\partial Z} + \left[\frac{\hbar^2}{\mu} K_F(K_F - k_F) + V_{FF}(\rho, Z) \right] C_F(\rho, Z) =$$

$$\sum_{n=1}^N C_n(\rho, Z) V_{Fn}(\rho, Z) \exp i(k_i - k_F) Z, \quad f = 1, 2, \dots, N \quad (13)$$

to be solved subject to the boundary condition $C_F(\rho, -\infty) = \delta_{iF}$. The above equations (8) - (13) are basic to the present multichannel eikonal treatment and a variety of approximations readily follow. For example, in the absence of all couplings except that connecting the initial and final channels i.e.

$C_n = \delta_{ni}$ in (13), then (8) reduces to

$$f_{if}(\theta, \phi) = -\frac{1}{4\pi} \frac{2\mu}{h} \int \tilde{V}_{fi}(\tilde{R}) \exp(i\tilde{K} \cdot \tilde{R}) d\tilde{R} \quad (14)$$

which is the Born-wave formula for the scattering amplitude.

When $K_f(\underline{R})$ is approximated by $k_f - \frac{u}{\hbar k_f} V_{ff}(\underline{R})$ then, with the aid of (6) for k_f^2 , both I_2 and the term within square brackets of LHS of (13) vanish identically to give,

$$r_{if}^A(\theta, \varphi) = -i^{\Delta+1} \int_0^\infty J_\Delta(K\rho) \rho d\rho \int_{-\infty}^\infty K_f \left(\frac{\partial C_f^A}{\partial Z} \right) \exp(i\alpha Z) dZ, \quad (15)$$

an approximation A to the scattering amplitude, for which the N-coupled equations reduce to

$$\frac{i\hbar^2}{u} K_f \frac{\partial C_f^A}{\partial Z} = \sum_{n=1}^N C_n^A(\rho, Z) V_{fn}(\rho, Z) \exp i(k_n - k_f)Z, \quad f = 1, 2, \dots, N$$

If the local wavenumber K_f in (15) and (16) is now replaced by its asymptotic value k_f then a further approximation B is obtained. For a one-channel approximation B, $C_n^B = C_i^B \delta_{in}$ in (16) with $K_i = k_i$. After some analysis, the customary Eikonal expression²² for elastic scattering by a fixed potential $V_{ii}(\underline{R})$ is then recovered. Moreover, if the distorted wave for the final state

$$\psi_f(\underline{r}, \underline{R}) = \phi_f(\underline{r}_1, \underline{r}_2) \exp i(k_f \cdot \underline{R} - \frac{i}{\hbar v_f} \int_{-\infty}^Z V_{ff} dZ) \quad (17)$$

is used in (1), then the theory follows through as before, to give, in approximation

$$r_{if}^{DW}(\theta, \varphi) = -i^{\Delta+1} \int_0^\infty J_\Delta(K\rho) \rho d\rho \int k_f \left(\frac{\partial C_f^B}{\partial Z} \right) \exp i \left(\alpha Z + \frac{1}{\hbar v_f} \int_{-\infty}^Z V_{ff} dZ' \right) dZ \quad (18)$$

where, C_f^B satisfies (16) with $K_f = k_f$. Eq. (18) represents

the multichannel distorted-wave treatment. By setting $C_n^B = C_i^B \delta_{in}$ in a two-

state treatment of (16) then, after some analysis, (18) reduces to

$$f_{if}^{DWB}(\theta, \varphi) = -\frac{i\Delta_{ii}}{\hbar^2} \int_0^\infty J_\Delta(k_F \rho \sin \theta) \rho \, d\rho \int_{-\infty}^\infty V_{fi}(\rho, Z) \times \exp i \left[\{ (k_i - k_F) + \alpha \} Z + \delta\bar{\phi}(Z) \right] dZ \quad (19)$$

where

$$\delta\bar{\phi}(Z) = -\frac{1}{\hbar v_i} \int_{-\infty}^Z V_{ii} dZ - \frac{1}{\hbar v_F} \int_Z^\infty V_{ff} dZ, \quad (20)$$

formulae which are identical to the distorted Born-wave expressions of Chen et al.²³ for e-H collisions. The above equations (19-20) have been used by Shields and Peacher²⁴ to evaluate differential cross sections for atom-atom collisions.

In the heavy-particle or high-energy limit, the asymptotic wavenumbers k_F in approximation B can be replaced by

$$k_F = k_i - \frac{e_{fi}}{\hbar v_i} \left(1 + \frac{e_{fi}}{2\mu v_i} + \dots \right), \quad e_{fi} = e_f - e_i \quad (21)$$

and a third approximation C(α) follows by setting all the individual k_n in Approximation B equal to k_i , and any difference $k_n - k_F = e_{fn}/v_i$. Hence

$$f_{if}^c(\theta, \varphi) = -i\Delta_{ii}^{+1} \int_0^\infty J_\Delta(k_i \rho) \left[\int_{-\infty}^\infty \frac{\partial C_F^c(\rho, Z)}{\partial Z} \exp(i\alpha Z) dZ \right] \rho \, d\rho, \quad \alpha = K_Z - \frac{e_{fi}}{\hbar v_i} \quad (22)$$

In addition, for small angle scattering at high energies $\alpha \approx 0$ from (11) and the Z-integration above can therefore be performed so that a further approximation $C(\alpha = 0)$ is characterized by

$$f_{if}^{c(0)}(\theta, \varphi) = -i^{\Delta+1} k_i \int_0^\infty J_\Delta(K'\rho) [C_f^c(\rho, \infty) - \delta_{if}] \rho d\rho \quad (23)$$

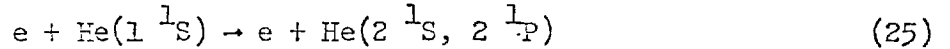
where $K'^2 = K^2 - e_{fi}^2/n^2 v_i^2$ and where the amplitudes C_f^c satisfy

$$i\hbar v_i \frac{\partial C_f^c}{\partial Z} = \sum_{n=1}^N C_i^c(\rho, Z) v_{fn}(\rho, Z) \exp\left(\frac{i e_{fn} Z}{\hbar v_i}\right) \quad (24)$$

in which $v_i = \hbar k_i / \mu$ for $n = 1, 2, \dots, N$, is the incident speed. These equations (22) - (24) are simply those derived previously²⁵ for the differential cross sections in the multistate impact parameter description of heavy particle collisions. They have recently been applied to various atom-atom and ion-atom collisions²⁶. Eq. (22) has previously been obtained by Byron⁵ who subsequently applied (23) and (24) to e - H(1s) collisions. In order to acknowledge polarization of the initial state due to the incident electron, Bransden and Coleman²⁷ modified (24) and used (23) with $K' = 2k_i \sin \frac{\theta}{2}$. The above derivation however demonstrates that the validity of the impact parameter equations (22-24) is confined only to the heavy-particle or high-energy limit of atomic collisions when $k_i \approx k_f$ and the scattering is mainly in the forward direction.

3. Results and Discussion

The full multichannel eikonal theory as represented by equations (8)-(13) is now applied to the examination of differential and total cross sections for the excitation processes



in which the four-channels $e - (1^1\text{S}, 2^1\text{S}, 2^1\text{P}_{0,\pm 1})$ of the e-He system are closely coupled. For this investigation two relevant orthogonal sets of wavefunctions were adopted. The first set includes the normalized Hartree-Fock ground-state function of Byron and Joachain²⁸,

$$\varphi_{1s,1s}(\underline{r}_1, \underline{r}_2) = \frac{1.6956}{\pi} \left[e^{-1.4r_1} + 0.799e^{-2.61r_1} \right] \left[e^{-1.4r_2} + 0.799e^{-2.61r_2} \right],$$

the 2^1P function of Goldberg and Clogston²⁹,

$$\varphi_{1s,2p}(\underline{r}_1, \underline{r}_2) = \frac{0.37831}{\pi^{\frac{3}{2}}} \left[r_1 e^{-(0.485r_1+2r_2)} Y_{1m}(\hat{r}_1) + r_2 e^{-(0.485r_2+2r_1)} Y_{1m}(\hat{r}_2) \right]$$

and the 2^1S function of Flannery⁷

$$\varphi_{1s,2s}(\underline{r}_1, \underline{r}_2) = \frac{0.70640}{\pi(1+\Delta)^{\frac{3}{2}}} \left[e^{-2r_2} (e^{-\lambda r_1} - c r_1 e^{-\mu r_1}) + e^{-2r_1} (e^{-\lambda r_2} - c r_2 e^{-\mu r_2}) \right]$$

in which the following parameters $\lambda = 1.1946$, $\mu = 0.4733$, $c = 0.26832$ and $\Delta = 0.007522$ which ensured orthogonality with (26) were chosen so as to provide a simple curvefit to the multi-parameter function of Cohen and McEachran³⁰.

With the aid of standard integral techniques, the interaction potentials (7), deduced from the above set of wavefunctions (26)-(28), can be expressed as analytic functions of R .

The second choice of wavefunctions are the actual analytical multi-parameter Hartree-Fock frozen-core set of McEachran and Cohen³¹ and of Crothers and McEachran³², which yield very accurate eigenenergies. The set is written as,

$$\psi_{ls,n\ell m}(\underline{r}_1, \underline{r}_2) = N_{n\ell} [\varphi_0(\underline{r}_1) \varphi_{n\ell m}(\underline{r}_2) + \varphi_0(\underline{r}_2) \varphi_{n\ell m}(\underline{r}_1)] \quad (30a)$$

where the normalized function representing the frozen ls orbital is

$$\varphi_0(\underline{r}) = 2^{5/2} e^{-2r} Y_{00}(\hat{r}) \quad (30b)$$

and where the unnormalized orbital for the second electron in state $(n\ell m)$ is, in atomic units,

$$\varphi_{n\ell m}(\underline{r}) = \sum_{j=2\ell+1}^{J=10} a_j^{n\ell} (2r)^\ell e^{-\beta r} L_j^{2\ell+1}(2\beta r) Y_{\ell m}(\hat{r}), \quad \beta = \frac{2}{n} \quad (30c)$$

where the coefficients $a_j^{n\ell}$ of the associated Laguerre polynomials

$$L_j^\lambda(x) = \sum_{k=0}^{j-\lambda} \frac{(-1)^{k+1} (j!) x^k}{k! (j-k-\lambda)! (k+\lambda)!} \quad (30d)$$

have been tabulated³⁰⁻³² for various states of helium. In order to evaluate the interaction matrix elements (7) as analytic functions of R , it is convenient to express (30c), with the aid of (30d) as

$$\varphi_{n\ell m}(\underline{r}) = \sum_{N=\ell+1}^{j-\lambda} \frac{B_N^{n\ell}}{N} e^{-\beta r} r^{N-1} Y_{\ell m}(\hat{r}) \quad (31a)$$

with coefficients given by

$$B_n^{n\ell} = \sum_{j=N+\ell}^J \frac{(-1)^{N-\ell} a_j^{n\ell} 2^\ell (j!)^2 (2\beta)^{N-\ell-1}}{(n-\ell-1)! (j-N-\ell)! (N+\ell)!} \quad (31b)$$

which are tabulated in table 1 for the 1^1S , 2^1S and 2^1P states of interest. The overall normalization factor in (30a) is $N_{n\ell} = [2(H_{n\ell} + G_{n\ell}^2)]^{-\frac{1}{2}}$ where

$$H_{n\ell} = \sum_{N=\ell+1}^{J-\ell} \sum_{N'=\ell+1}^{J-\ell} B_N^{n\ell} B_{N'}^{n\ell} \frac{(N+N')!}{(2\beta)^{N+N'+1}} \quad (31c)$$

and

$$G_{n\ell} = 2^{5/2} \delta_{\ell 0} \sum_{N=1}^J B_N^{n\ell} \frac{(N+1)!}{(\beta+2)^{N+1}} \quad (31d)$$

and is also given in table 1. With the aid of (31a)-(31b), and standard integrals, the interaction matrix elements can be expressed in the form

$$V_{n\ell m, n'\ell' m'}^{(R)} = \sum_{L=| \ell-\ell' |}^{| \ell+\ell' |} \left[-\frac{a_{-t}}{R^t} + \sum_{i=1}^2 e^{-\alpha_i R} \sum_{s=-t}^{16} a_s R^s \right] Y_{LM}(\tilde{R}) \quad (32)$$

The tabulation of the coefficients a_m for the various $\alpha_i = 4$ and $(1/n + 1/n')$, and L values is extensive and is available upon request. With a knowledge of the interaction matrices (32), the appropriate set of coupled differential equations (15) can be solved for the real and imaginary parts of C_i by standard numerical procedures.

In figs. (1-2), the resulting differential cross sections,

$$\frac{d\sigma}{d\Omega} = \frac{k_f}{k_i} |f_{if}(\theta, \phi)|^2 \quad (33)$$

computed from (8)-(13) as a function of scattering angle θ are displayed as solid and double-dashed curves (labelled FE1 and FE2 associated with the first and second choices (26-28) and (30a-30d) for the wavefunctions respectively) at two representative electron-impact energies E_i of 50 eV and 100 eV. Use of the more refined set of wavefunctions (30a-30d) causes the scattering to be increased only in the forward direction ($\theta \lesssim 20^\circ$) in the case of 2^1P excitation, and into all angles for the 2^1S collision. This amount of enhancement decreases with energy-increase. Also shown are recent results labelled S, single-dashed curves, obtained by Berrington et al.³³ who used the first set of orthogonal wavefunctions (26-28) in the second-order potential theory of Bransden and Coleman²⁷, i.e. equations (23) with $K' = 2k_i \sin \frac{\theta}{2}$ and (24) suitably modified so as to acknowledge polarization of the initial state. While the long-range polarization is expected to be more effective for small-angle scattering (i.e. distant encounters), Berrington et al.³³ have shown that the resulting reduction in $d\sigma/d\Omega$ is nonetheless relatively small at small θ and vanishes for larger θ and/or E_i . Figs. (1a-1b) show that the present treatment causes a further reduction both at small and large scattering angles for the 2^1P excitation. In figs. (2a-b) the effect is reversed for the 2^1S excitation. These effects can be attributed to the presence in (9) and (10) of α which tends to reduce all the cross sections particularly at the larger scattering angles and to the more important inclusion in the various channels of the different local momenta $K_n(R)$ which tend to enhance²¹ the 2^1S excitation at the expense of the 2^1P excitation at energies $\gtrsim 50$ eV.

The 2^1P and 2^1S differential cross sections measured by various groups^{4,15-19} are also displayed in the figs. (1-2) for comparison purposes. Although large discrepancies do exist between the measured values particularly for scattering

at all angles for 50 eV, and for large-angle scattering, in general, the overall agreement with theory is satisfactory only for scattering into small and intermediate angles $\lesssim 50^\circ$.

While the present treatment includes several important effects e.g. the $2^1P - 2^1S$ coupling and the different relative local momenta in the various channels, it ignores both electron-exchange and that additional part of the polarization-interaction in the incident channel not included via the four-state treatment. Electron-exchange is mainly effective at the large scattering angles (i.e. close encounters) while the long-range polarization attraction mainly affects elastic scattering in the forward direction. For e-H(1s) excitation at 50 eV, Chen et al.²⁵ have shown the exchange effect to be small for $\theta \lesssim 30^\circ$, an effect which is entirely dominated by the more important 2p-2s coupling included by Flannery and McCann²¹, but neglected in the treatment of Chen et al.²³ According to Berrington et al.³³, the neglect of the additional amount of polarization in the incident channel introduces relatively small error³³ for e-He inelastic scattering in the forward direction. The present theoretical formulation is however amenable to the inclusion of both electron-exchange and the full polarization interaction.

In figs. (3a)-(3b) are displayed the theoretical cross sections together with other theoretical values and the measurements for the total 2^1P excitations, refs. (9-12), and for the 2^1S excitations, refs. (13-15). Donaldson et al.⁹ normalized their experimental data to the Born cross sections at 2000 eV. As exhibited in the figures, the present theory represents considerable improvement over the Born B and the second-order potential treatments, although a great deal of scatter still exists in the experimental data. The theoretical prediction

of a peak in the 2^1P excitation around 80 eV is consistent with the experimental data. The use of the less accurate wavefunctions (26-28) reduces the 2^1P and 2^1S (FE2) cross sections by 6% and 12% respectively. Comparison of FE1 and S in figure (3b) shows that the additional physical effects acknowledged by the present treatment for the 2^1S excitation has introduced closer accord with experiment, while comparison between FE2 and FE1 demonstrate the need for using wavefunctions as accurate as possible. It is worth noting that the present Hartree-Fock frozen core set of wavefunctions are the most accurate employed to date in a collision description more refined than Born's approximation.

In tables 2 and 3 are displayed the actual numerical $2^1P_{0,\pm 1}$ and 2^1S excitation cross sections FE2, together with those given by Born's approximation B, the four-state impact treatment IP and the second-order potential method S. For the 2^1P excitation at impact energies $E_i \lesssim 200$ eV, IP and S are higher than B which at 50 eV is in turn higher than the present four-state eikonal results FE2 by 34%. For the 2^1S excitation all the cross sections are lower than Born's approximation and the use of the more accurate second set of wavefunctions (30a) has resulted in (fortuitous) closer accord with IP and S which were determined from wavefunctions (26)-(28). At 500 eV, the Born cross sections are 3% and 6% higher than the FE2 results for the 2^1P and 2^1S excitations respectively.

Also tabulated in table 2 is the percentage polarization P of the radiation emitted from the 2^1P level obtained from the formula³⁴

$$P = \frac{100(\sigma_0 - \sigma_1)}{\sigma_0 + \sigma_1} \quad (34)$$

where σ_m is the cross section for excitation of a particular substate m. Direct measurement of P for a vacuum UV emission is extremely difficult.

In conclusion, the theoretical acknowledgment of the different local wavenumbers $K_n(R)$ eqn. (6) of relative motion in various channels, the important $2^1P - 2^1S$ dipole coupling, the momentum parameter α eq. (11), and various distortion effects within a multichannel eikonal treatment of atomic collisions has introduced closer accord with experiment for e - He collisions and in particular has produced a theoretical peak absent in previous theoretical treatments of the 2^1P cross section. The effect of including these physical effects can however be rendered null for the 2^1S excitation by an inappropriate choice of wavefunctions, i.e. the inclusion of refinements to the collision theory should be preferably accompanied, whenever possible, by a choice of accurate He-wavefunctions. The present agreement for e-He($1s^2$) collisions taken together with the previous²¹ agreement for e-H($1s$) collisions is encouraging and represents the status of the present multichannel eikonal approximation. In particular, this theoretical model finds ready application over a large impact energy range to e-excited atom and e-complex atom collisions, instances for which application of the full wave treatment is prohibitively difficult.

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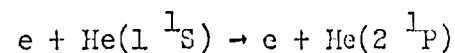
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Table 1: Coefficients B_N , parameters β , normalization factors N_{nl} and eigenenergies ϵ_n (a.u) given by the Hartree-Fock frozen core set of wavefunctions (30a-31a) for helium.

$N \backslash B_N$	1s	2s	2p
1	-1.8385(0)*	-5.5677(-1)	0.0000
2	2.9332(-2)	5.2732(-1)	-1.2768(-1)
3	-1.2332(0)	-4.1053(-1)	-5.8948(-2)
4	-4.7143(-3)	3.1444(-1)	-1.5165(-2)
5	1.0769(-1)	-9.0158(-2)	-1.3793(-2)
6	-7.9926(-2)	1.7266(-2)	4.9854(-3)
7	2.0400(-2)	-1.5858(-3)	-1.2073(-3)
8	-2.6249(-3)	7.3009(-5)	1.1661(-4)
9	1.2433(-4)	-3.0679(-7)	-5.2312(-6)
β	2.0	1.0	1.0
N_{nl}	2.2745	9.1927(-2)	3.6218(-2)
ϵ_n (calc)	-0.8725	-0.1434	-0.1224
ϵ_n (expt)	-0.9036	-0.1460	-0.1238

* The number in parentheses indicates the power of ten by which the entry is to be multiplied.

Table 2. Inelastic Cross Sections (πa_0^2) for the Process



E_i (eV)	FE^a				$2\ ^1\text{P}$		
	$2\ ^1\text{P}_0$	$2\ ^1\text{P}_{\text{all}}$	$2\ ^1\text{P}$	P^e	S^b	$1P^c$	Born ^d
50	0.0732	0.0600	0.1332	41.9	0.215	0.232	0.1694
80	0.0637	0.0750	0.1387	25.9	--	--	0.1596
100	0.0547	0.0759	0.1306	18.1	0.155	0.161	0.1485
200	0.0347	0.0671	0.1018	1.7	0.105	0.107	0.1069
300	0.0237	0.0577	0.0814	-9.8	0.0822	0.083	0.0841
400	0.0173	0.0500	0.0673	-18.2	0.0681	0.069	0.0700
500	0.0120	0.0466	0.0586	-32.0	0.0581	0.058	0.0602

a: Present four-channel eikonal treatment (refined set of wave functions, eqns. 30a-30d).

b: Second-order potential method (Berrington et al.³³).

c: Impact-Parameter method (Berrington et al.³³).

d: Born approximation (Bell et al.²)

e: Percentage polarization of emitted radiation.

Table 5. Inelastic Cross Sections (πa_0^2) for the Process
 $e + \text{He}(1^1\text{S}) \rightarrow e + \text{He}(2^1\text{S})$

E_i (eV)	FE ^a	S ^b	IP ^c	Born ^d
50	0.0215	0.0225	0.031	0.0390
60	0.0175	--	--	0.0270
100	0.0155	0.0154	0.0182	0.0222
200	0.0096	0.0093	0.0102	0.0118
300	0.0070	0.0066	0.0071	0.0080
400	0.0054	0.0052	0.0054	0.0060
500	0.0045	0.0042	0.0044	0.0048

a: Present four-channel treatment (refined set of wave functions, eqns. 30a-30d).

b: Second-order potential method (Berrington et al.³³).

c: Impact-Parameter method (Berrington et al.³³).

d: Born approximation (Bell et al.²):

FIGURE CAPTIONS

Figure 1. Differential cross sections for the process $e + \text{He}(1^1\text{S}) \rightarrow e + \text{He}(2^1\text{P})$ at incident electron energy (a) 50 eV and (b) 100 eV.

Theory: FE1: Four channel eikonal treatment with first set of atomic wavefunctions (26)-(28).
FE2: Four channel eikonal treatment with second set of atomic wavefunctions (30).
S: Second-Order potential method with first set of atomic wavefunctions (Berrington et al.³²).

Experiment: Δ : Chamberlain et al.¹⁷
 \times : Crooks and Rudd¹⁸.
 \bullet : Truhlar et al.¹⁹ at 55.5 eV and Vriens et al.¹⁵ at 100 eV.

Figure 2. Differential cross sections for the process $e + \text{He}(1^1\text{S}) \rightarrow e + \text{He}(2^1\text{S})$ at incident electron energy (a) 50 eV and (b) 100 eV.

Theory: FE1: Four channel eikonal treatment with first set of atomic wavefunctions (26)-(28).
FE2: Four channel eikonal treatment with second set of atomic wavefunctions (30).
S: Second-Order potential method with first set of atomic wavefunctions (Berrington et al.³²).

Experiment: SM: Simpson et al.¹⁶
 Δ : Chamberlain et al.¹⁷
 \times : Crooks and Rudd¹⁸
 \bullet : Rice et al.⁴ at 55.5 eV and Vriens et al.¹⁵ at 100 eV.

Figure 3. Total cross sections for (a) the 2^1P and (b) the 2^1S excitations of $\text{He}(1^1\text{S})$ by electron impact.

Theory: FE1: Four channel eikonal treatment with first set of atomic wavefunctions (26)-(28).
FE2: Four channel eikonal treatment with second set of atomic wavefunctions (30).
S: Second-Order potential method with first set of atomic wavefunctions (Berrington et al.³²).
B: Born-approximation².

Experiment: (2^1P): Δ : Donaldson et al.⁹
 \square : Jobe and St. John¹⁰
 \times : Moustafa-Moussa¹¹.
 \bullet : van Eck and de Jongh¹²
(2^1S): Δ : Lassetre et al.¹³
 \times : Miller et al.¹⁴
 \bullet : Vriens et al.¹⁵

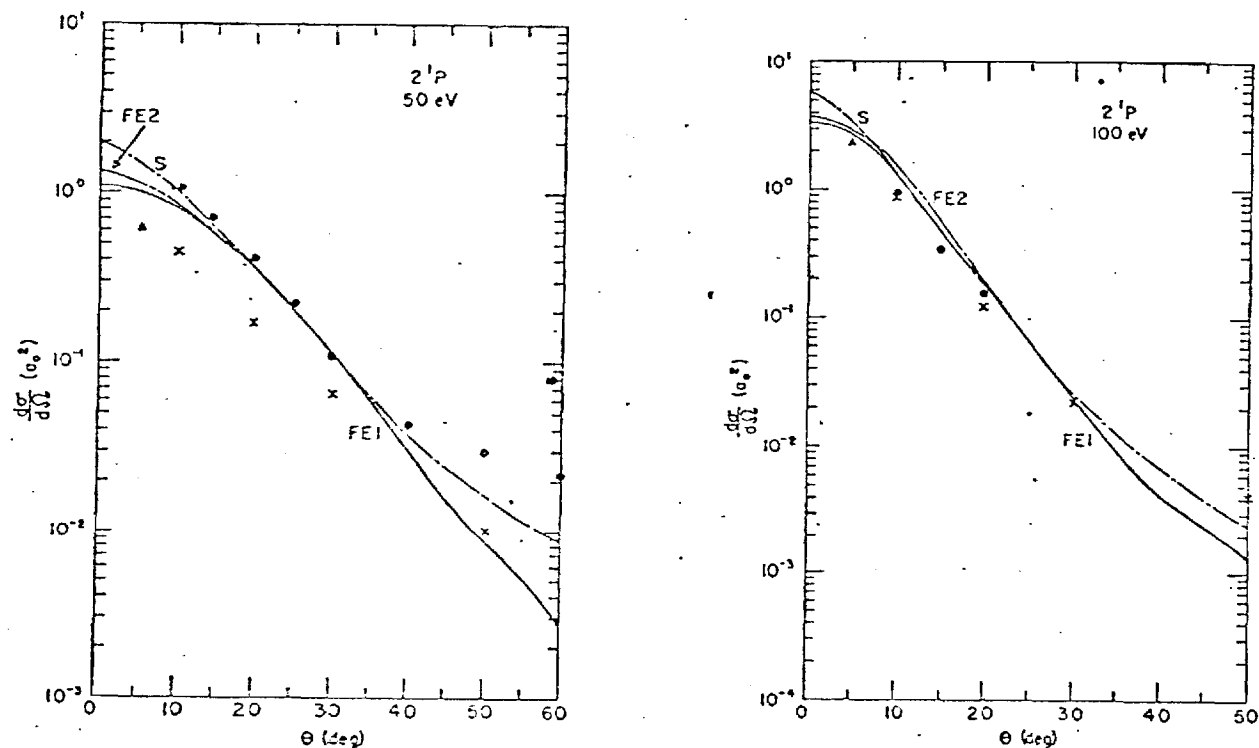


Figure 1. Differential cross sections for the process $e + \text{He}(1^1\text{S}) \rightarrow e + \text{He}(2^1\text{P})$ at incident electron energy (a) 50 eV and (b) 100 eV.

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 FE2: Four channel eikonal treatment with second set of atomic wavefunctions (30).
 S: Second-Order potential method with first set of atomic wavefunctions (Berrington et al.³²).

Experiment: Δ : Chamberlain et al.¹⁷
 \times : Crooks and Rudd¹⁸.
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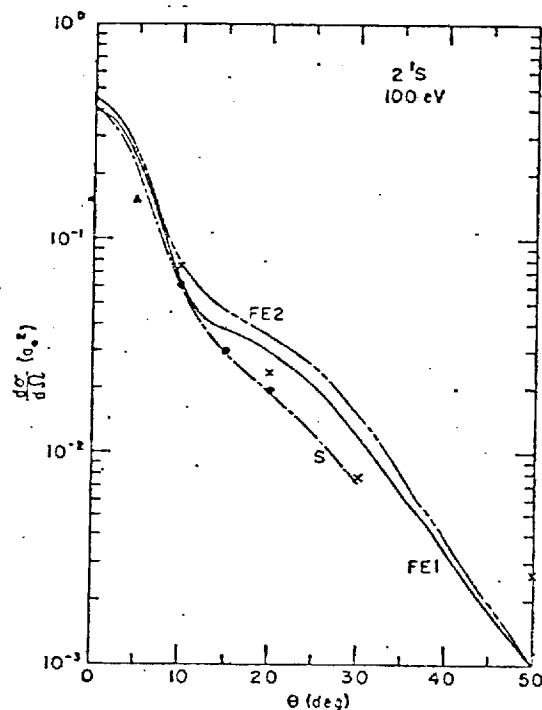
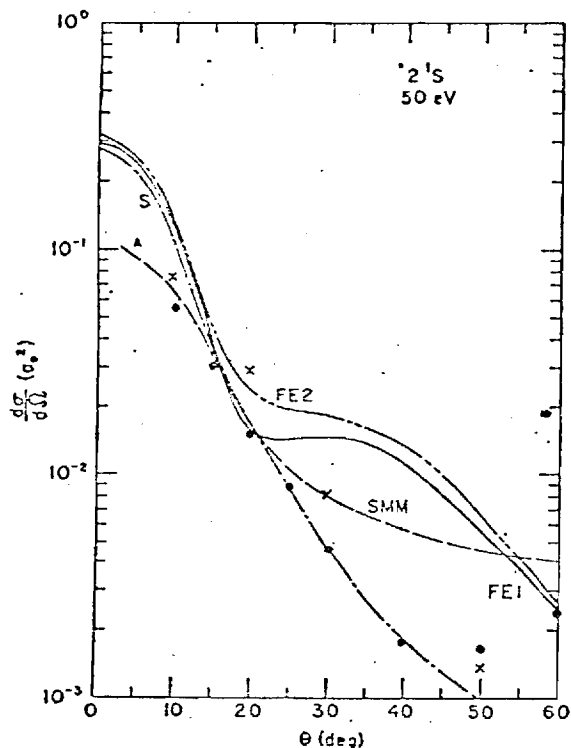


Figure 2. Differential cross sections for the process $e + \text{He}(1^1\text{S}) \rightarrow e + \text{He}(2^1\text{S})$ at incident electron energy (a) 50 eV and (b) 100 eV.

Theory: FE1: Four channel eikonal treatment with first set of atomic wavefunctions (26)-(28).

FE2: Four channel eikonal treatment with second set of atomic wavefunctions (30).

S: Second-Order potential method with first set of atomic wavefunctions (Berrington et al.³²).

Experiment: SSK: Simpson et al.¹⁶

Δ: Chamberlain et al.¹⁷

X: Crooks and Rudd¹⁸

○: Rice et al.⁴ at 55.5 eV and Vriens et al.¹⁵ at 100 eV.

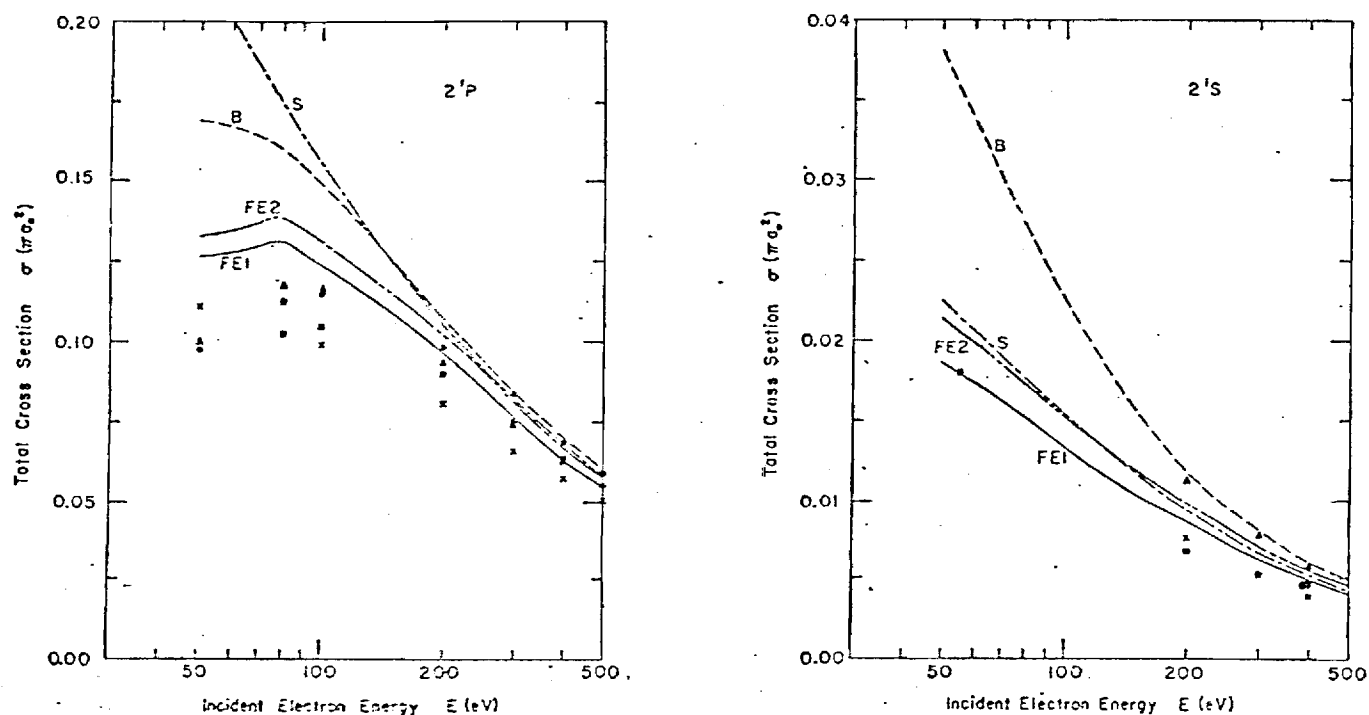


Figure 5. Total cross sections for (a) the 2^1P and (b) the 2^1S excitations of $\text{He}(1^1S)$ by electron impact.

Theory: FE1: Four channel eikonal treatment with first set of atomic wavefunctions (26)-(28).
 FE2: Four channel eikonal treatment with second set of atomic wavefunctions (30).
 S: Second-order potential method with first set of atomic wavefunctions (Berrington et al.²³).
 B: Born-approximation².

Experiment: (2^1P): Δ : Donaldson et al.⁹
 \square : Jobe and St. John¹⁰
 \times : Moustafa-Moussa¹¹.
 \circ : van Eck and de Jongh¹²
 (2^1S): Δ : Lassette et al.¹³
 \times : Miller et al.¹⁴
 \circ : Triens et al.¹⁵

APPENDIX B: The Multichannel Treatment of Atomic Collisions.

(To appear in abstracts of "International Conference
on electron and photon interactions with Atoms", and
"The Fourth International Conference on Atomic Physics".)

The Multichannel Eikonal Treatment of Atomic Collisions

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A variety of methods have been proposed for the theoretical description of e-atom collisions at low and intermediate energies. The close coupling expansion¹ with its pseudo-state modifications, and the polarized orbital distorted wave model of McDowell et al.² are among those that follow from the full wave treatment of the collisions. Other methods, termed as semiclassical - the Eikonal Approximations of Byron³ and of Chen et al.⁴, the impact parameter approach⁵, and the Glauber approximation⁶ - all essentially separate the relative motion of the incident electron (described by a eikonal-type or Born wavefunction for the electron in a static field) from the internal electronic motions of the atomic system which is described by a multistate expansion.

In this paper, a new generalization of the Eikonal approach to atomic collisions is developed. The relative motion is coupled with the electronic motions and the treatment accounts explicitly for the changes in speed associated with the various channels and for other effects not acknowledged by the previous semiclassical descriptions. The main advantages associated with such a treatment are: (a) its capability of systematic improvement in that multichannel couplings, electron-exchange and polarization effects can be explicitly acknowledged and (b) its application with relative ease to e-excited atom collisions which are important to the analysis of gaseous-discharges, laser development and astrophysical problems as well as to collisions involving complex atoms.

By following the multichannel Eikonal description of atomic collisions, it can be shown that the amplitude for scattering with final relative momentum \underline{k}_f in direction (θ, φ) with respect to polar axis along the direction of incident relation momentum \underline{k}_i is⁷

$$f_{if}(\theta, \varphi) = -i^{\Delta+1} \int_0^\infty J_\Delta(K'\rho) [I_1(\rho, \theta) - i I_2(\rho, \theta)] \rho d\rho \quad (1)$$

where J_Δ are Bessel functions of integral order, and where K' is the XY-component $k_f \sin \theta$ of the momentum-change $\underline{K} = \underline{k}_i - \underline{k}_f$.

The collisions functions

$$I_1(\rho, \theta; \alpha) = \int_{-\infty}^{\infty} \kappa_f(\rho, Z) \left[\frac{\partial C_f(\rho, Z)}{\partial Z} \right] \exp(i\alpha Z) dZ \quad (2)$$

and

$$I_2(\rho, \theta; \alpha) = \int_{-\infty}^{\infty} \left[\kappa_f(\kappa_f - k_f) + \frac{\mu}{h^2} V_{ff} \right] C_f(\rho, Z) \exp(i\alpha Z) dZ \quad (3)$$

contain a dependence on the scattering angle θ via

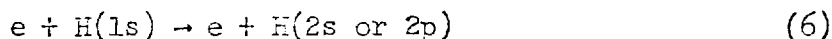
$$\alpha = k_f(1 - \cos \theta) = 2k_f \sin^2 \frac{\theta}{2} \quad (4)$$

the difference between the Z-component of the momentum change \tilde{K} and the minimum change $k_i - k_f$ in the collision. The coupling amplitudes C_f are solutions of the following set of N-coupled linear equations

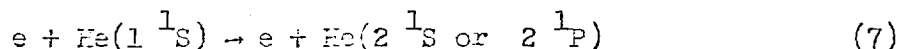
$$\begin{aligned} & \frac{h^2}{\mu} \kappa_f(\rho, Z) \frac{\partial C_f(\rho, Z)}{\partial Z} + \left[\frac{h^2}{\mu} \kappa_f(\kappa_f - k_f) + V_{ff}(\rho, Z) \right] C_f(\rho, Z) = \\ & \sum_{n=1}^N C_n(\rho, Z) V_{fn}(\rho, Z) \exp i(k_i - k_f) Z, \quad f = 1, 2, \dots, N \end{aligned} \quad (5)$$

solved subject to the boundary condition $C_f(\rho, -\infty) = \delta_{if}$. The local wavenumber of relative motion at separation $\tilde{R} \equiv (R, \Theta, \Phi) \equiv (\rho, \theta, Z)$ is $\kappa_n(\tilde{R}) = [k_n^2 - \frac{2\mu}{h^2} V_{nn}(\tilde{R})]^{\frac{1}{2}}$ where the interaction matrix elements $V_{nm}(\tilde{R}) = \langle \phi_n(\tilde{r}) | V(\tilde{r}, \tilde{R}) | \phi_m(\tilde{r}) \rangle$ connect the various electronic states $\phi_n(\tilde{r})$ describing the isolated systems and where $V(\tilde{r}, \tilde{R})$ is the instantaneous electrostatic interaction. It can be shown⁷ that successive approximation to the above equations (1)-(5) yields formulae previously derived.³⁻⁶

In figures (1a,b) and (2a,b) are shown excitation cross sections calculated from the above theory for the processes



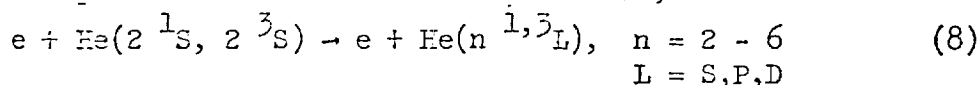
and



in which four electron-atom channels are closely coupled. The agreement between the present results and other refined treatments^{1,2,8,9} and various experiments¹⁰⁻¹⁸ is impressive. The differential cross

sections show similar accord and will be presented at the conference.

We also hope to provide detailed cross sections for,



excitation processes of profound importance in gaseous discharges and astrophysical plasmas.

Acknowledgement: This research was sponsored by the Air Force Aerospace Research Laboratories, Air Force Systems Command, United States Air Force, Contract F 33615-74-C-4003.

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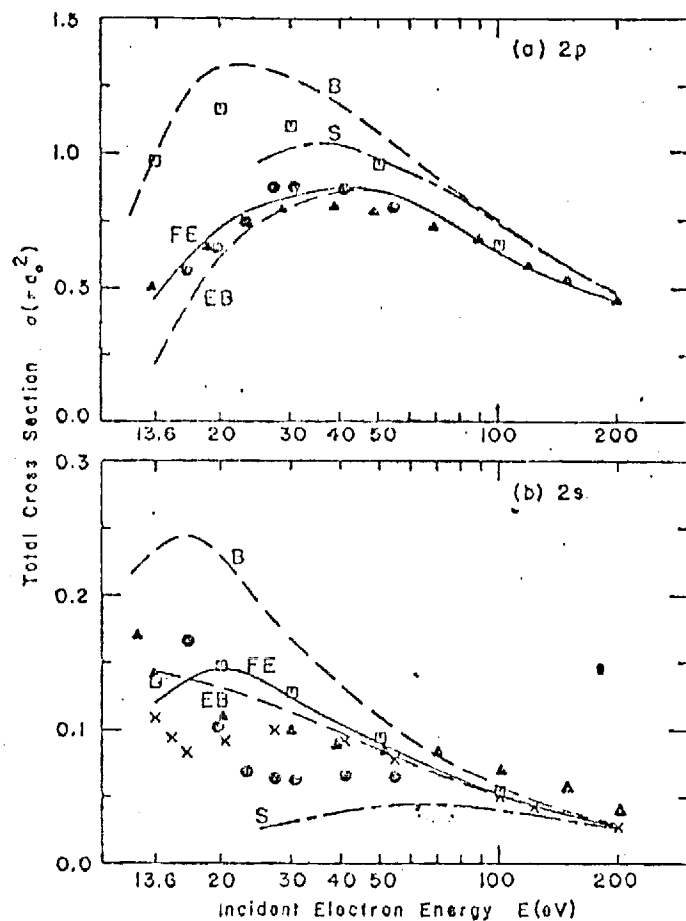


Figure 1: Cross sections for the 2p and 2s excitations of $H(1s)$ by electron impact. Theory: FE, full eikonal treatment; EB, eikonal approximation $B(X_n = k_n)$; S, second-order potential method; B, Born approximation; \odot , pseudo-state method; X, polarized-orbital distorted wave model; \square , four-state impact-parameter method; Experiment: Δ .

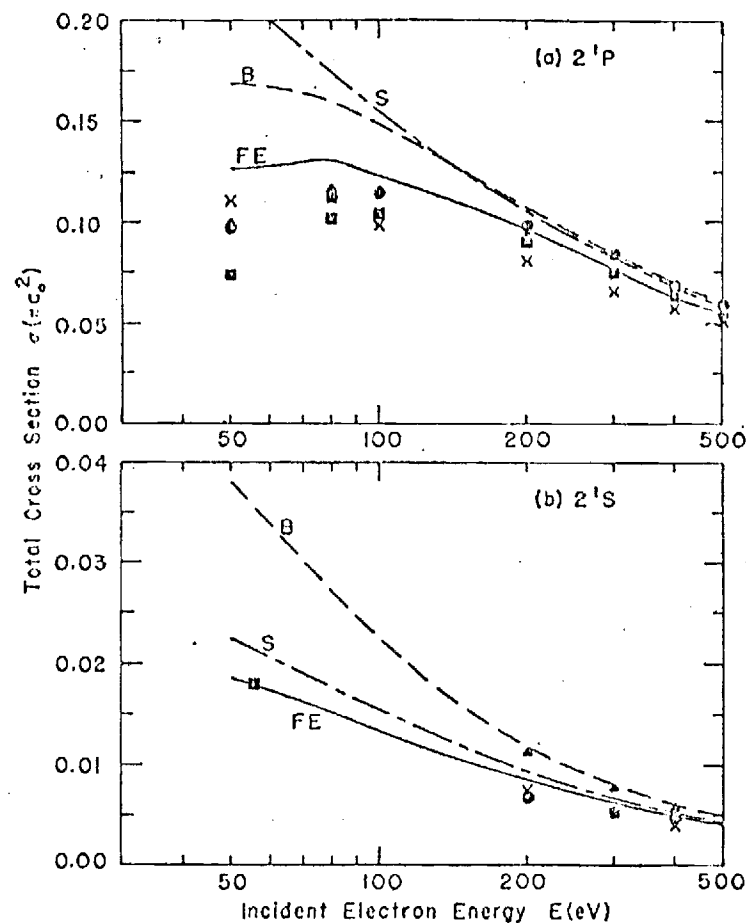


Figure 2: Cross sections for the 2^1P and 2^1S excitations of $He(1^1S)$ by electron impact. Theory: FE, full eikonal treatment; S, second-order potential method; B, Born approximation. Experiment (2^1P): Δ , Donaldson; X, Moustafa-Moussa; \odot , Van Eck; \square , Jobe. Experiment (2^1S): Δ , Lanzette; X, Miller; \odot , Vriens.

APPENDIX C: The Multichannel Treatment of Electron-atom Collisions.

(To appear in Proceedings of International Conference
on electron and photon interactions with atoms, in
honor of Ugo Fano, Plenum Press)

The Multichannel Eikonal Treatment of Electron-atom Collisions

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Abstract: A multichannel treatment of atomic collisions is presented and applied to the excitation of atomic hydrogen and helium by electrons with incident energy above the ionization threshold. The calculated cross sections compare very favorably with other refined theoretical procedures and with various experiments.

Short Title: Multichannel Eikonal Treatment

1. Introduction

A variety of methods have been proposed for the theoretical description of e-atom collisions at low and intermediate energies. The close coupling expansion with its pseudo-state modifications (Burke and Webb 1970), and the polarized orbital distorted wave model of McDowell et al. (1973) are among those that follow from the full wave treatment of the collision. Other methods, termed as semiclassical - the Eikonal Approximations of Bates and Holt (1966), Callaway (1968), Byron (1971) and of Chen et al. (1972), the impact parameter approach (Bransden and Coleman 1972), and the Glauber approximation (cf. Tai et al., 1972) - all essentially separate the relative motion of the incident electron (described by an eikonal-type or Born wavefunction for the electron in a static field) from the internal electronic motions of the atomic system which is described by a multistate expansion. In this paper, a new generalization of the Eikonal approximation to multichannel scattering is presented.

2. Theory

Consider the collision of a particle B of mass M_B and incident velocity \underline{v}_i along the Z-axis with a one electron atomic system (A + e) of mass ($M_A + m$). The subsequent analysis can be immediately generalized so as to cover multi-electron systems. Let \underline{R} , \underline{R}_B , \underline{r} and \underline{r}_A denote the A - B, B - (Ae) center of mass, e - (AB) center of mass, and e - A separations, respectively. In the (ABe) center-of-mass reference frame, the scattering amplitude for a direct transition between an initial state i and a final state f of the collision system, of reduced mass μ , is

$$f_{if}(\theta, \varphi) = -\frac{1}{2\pi} \frac{2\mu}{\hbar^2} \langle \psi_f(\underline{k}_f; \underline{r}, \underline{R}) | V(\underline{r}, \underline{R}) | \psi_i^+(\underline{k}_i; \underline{r}, \underline{R}) \rangle_{\underline{r}, \underline{R}} \quad (1)$$

in which $V(\underline{r}, R)$ is the instantaneous electrostatic interaction between the collisions species, and where the scattering is directed along the final relative momentum $\underline{k}_f(1, \theta, \phi)$. The final stationary state of the isolated atoms in channel i is ψ_i , and ψ_i^+ is the solution of the time independent Schrödinger equation,

$$\left[-\frac{\hbar^2}{2\mu} \nabla_R^2 + H_e(\underline{r}) + V(\underline{r}, R) \right] \psi_i^+(\underline{r}, R) = E_i \psi_i^+(\underline{r}, R) \quad (2)$$

solved subject to the asymptotic boundary condition,

$$\psi_i^+(\underline{r}, R) \xrightarrow{\text{large } R} \sum_n \left[e^{i\mathbf{k}_n \cdot \underline{R}} \delta_{ni} + f_{in}(\theta, \phi) \frac{e^{i\mathbf{k}_n \cdot \underline{R}}}{R_B} \right] \phi_n(\underline{r}_a) \quad (3)$$

in which $\phi_n(\underline{r}_a)$ are eigenfunctions of the Hamiltonian $H_e(\underline{r}) \approx H_e(\underline{r}_a)$ for the isolated atomic system $(A + e)$ with internal electronic energy ϵ_n such that the total energy E_i in channel i is $\epsilon_i + \hbar^2 k_i^2 / 2\mu$ which is conserved throughout the collision.

2.1 The Multichannel Eikonal Approximation

The Eikonal Approximation to (2) sets

$$\psi_i^+(\underline{r}, R) = \sum_n A_n(\rho, Z) \exp i S_n(\rho, Z) \phi_n(\underline{r}_a) \exp i \left(\frac{m}{M_A + m} \mathbf{k}_n \cdot \underline{r}_a \right) \quad (4)$$

where the nuclear separation $\underline{R} = (R, \Theta, \Phi) = (\rho, \phi, Z)$ in spherical and cylindrical coordinate frames respectively. The eikonal S_n in (4) is the characteristic-function solution of the classical Hamilton-Jacobi equation (i.e. the Schrödinger equation in the $\hbar \rightarrow 0$ limit) for the A - B relative motion under the static interaction $V_{nn}(\underline{R}) = \langle \phi_n | V | \phi_n \rangle$ and is therefore given by

$$S_n(\rho, Z) = k_n Z + \int_{-\infty}^Z [K_n(R) - k_n] dZ \quad (5)$$

in which the local wavenumber $K_n(R)$ of relative motion at R is $\left[k_n^2 - \frac{2\mu}{\hbar^2} V_{nn}(R) \right]^{\frac{1}{2}}$ and where dZ is an element of path length along the trajectory which, at present, is taken as a straight line. For electron-atom collisions, K_n in (6) is always real. The use of the actual classical trajectory with its 'built-in' turning point is therefore not as essential as in, for example, positron-atom collisions when K_n becomes imaginary for sufficiently close rectilinear encounters. The general problems associated with the choice of classical trajectory within a multichannel framework are at present unresolved, although the forced-common turning-point, two-state procedure of Bates and Crothers (1970) is attractive.

On assuming that the main variation of Ψ_i^+ on ρ is contained in S_n , i.e. provided $V_{nn}(R)$ varies slowly over many wavelengths $2\pi/K(R)$ of relative motion, and the coefficients $A_n(\rho, Z)$ therefore vary primarily along Z , then substitution of (4) in (2) yields the set of coupled differential equations,

$$\frac{i\hbar^2}{\mu} K_f \frac{\partial B_f(\rho, Z)}{\partial Z} + \left[\frac{\hbar^2}{\mu} K_f (K_f - k_f) + V_{ff}(R) \right] B_f(\rho, Z) = \quad (6)$$

$$\sum_{n=1}^N B_n(\rho, Z) V_{fn}(R) \exp i (k_n - k_f) Z, \quad f = 1, 2, \dots, N$$

a set of N coupled equations to be solved for $B_f = A_f \exp \left(i \int_{-\infty}^Z (K_f - k_f) dZ \right)$

subject to the asymptotic condition $B_f(\rho, -\infty) = \delta_{fi}$ which ensures that

$\Psi_i \sim \psi_i(r_2) \exp(ik_i Z)$ as $Z \rightarrow -\infty$. The scattering amplitude (1) with the

undistorted final wave $\psi_f = \psi_f(\underline{r}_2) \exp(i\mathbf{k}_f \cdot \underline{R})$ inserted, is therefore,

$$f_{if}(\theta, \varphi) = -\frac{1}{i\hbar} \frac{2u}{2} \int \exp(i\mathbf{K} \cdot \underline{R}) d\underline{R} \sum_{n=1}^N B_n(\rho, Z) V_{fn}(\underline{R}) \exp i(k_n - k_i)Z \quad (7)$$

where \mathbf{K} is the momentum change $\mathbf{k}_i - \mathbf{k}_f$ caused by the collision. Since the electrostatic interaction $V(\underline{r}, \underline{R})$ is composed of central potentials,

$V_{fi} = \langle \psi_f | V | \psi_i \rangle = V_{fi}(\underline{R}, \theta) \exp i \Delta \phi$, where $\Delta = M_i - M_f$ is the change in the azimuthal quantum number of the atom. Hence with the substitution $C_f(\rho, Z) = B_f(\rho, Z) \exp(-i \Delta \phi)$ the set of phase ϕ -independent equations

$$\frac{\hbar^2}{u} K_f(\rho, Z) \frac{\partial C_f(\rho, Z)}{\partial Z} + \left[\frac{\hbar^2}{u} K_f(K_f - k_f) + V_{ff}(\rho, Z) \right] C_f(\rho, Z) = \quad (8)$$

$$\sum_{n=1}^N C_n(\rho, Z) V_{fn}(\rho, Z) \exp i(k_n - k_f) Z$$

is obtained, solved subject to the boundary condition $C_f(\rho, -\infty) = \delta_{if}$. On completion of the ϕ -integration in (7), the scattering amplitude reduces to

$$f_{if}(\theta, \varphi) = -i^{\Delta+1} \int_0^\infty J_\Delta(K' \rho) [I_1(\rho, \theta) - i I_2(\rho, \theta)] \rho d\rho \quad (9)$$

where K' is the XY-component $k_f \sin \theta$ of \mathbf{K} and where J_Δ are Bessel functions of integral order. Both the functions

$$I_\pm(\rho, \theta; Z) = \int_{-\infty}^\infty K_f(\rho, Z) \left[\frac{\partial C_f(\rho, Z)}{\partial Z} \right] \exp(i\alpha Z) dZ \quad (10)$$

and

$$I_2(\rho, \theta; \alpha) = \int_{-\infty}^{\infty} \left[\tilde{K}_2(K_F - \frac{k_F}{n}) + \frac{\mu}{2} V_{ff} \right] C_F(\rho, Z) \exp(i\alpha Z) dZ \quad (11)$$

contain a dependence on the scattering angle θ via

$$\alpha = k_F(1 - \cos \theta) = 2k_F \sin^2 \frac{\theta}{2} \quad (12)$$

the difference between the Z-component of the momentum change \tilde{K} and the minimum momentum change $k_i - k_f$ in the collisions. Equations (8 - 12) are the basic formulae given by the present Multichannel Eikonal description for the scattering amplitude, and can be easily generalized so as to cover collisions involving multielectron systems. It is apparent that a variety of approximations readily follow. Note that in the absence of all couplings except that connecting the initial and final channels i.e. $C_n = \delta_{ni}$, then either (7) or (9) directly yields

$$a_{fi}(\theta, \theta) = - \frac{1}{4\pi} \frac{2\mu}{n} \int \tilde{V}_{fi}(\underline{R}) \exp(i\underline{K} \cdot \underline{R}) d\underline{R} \quad (13)$$

which is the Born-wave scattering amplitude.

Moreover, it can be shown (Flannery and McCann, 1974) by successive approximation, that the above equations can reproduce (a) the customary one-channel Eikonal expression (cf. Bransden, 1970) for elastic scattering and (b) the Distorted-Born wave expression of Chen et. al. (1972). Also, in the heavy-particle or high-energy limit the usual impact-parameter and Glauber formulae are recovered.

In summary, the present method

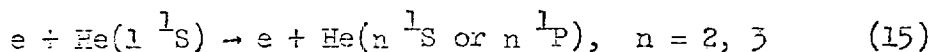
- (i) has defined a scattering amplitude rather than an excitation probability, the key quantity occurring in time-dependent impact-parameter treatments,
- (ii) has acknowledged different local momenta of relative motion in various channels, and
- (iii) has automatically included an infinite number of partial waves, via the Eikonal in (4), which are distorted by the static interactions associated with the various channels and which in turn are coupled to the internal electronic motions via A_n in (4).

3. Results and Discussion

As examples of the preceding analysis, the full Eikonal equations (8)-(12) are now applied to the examination of the excitation processes



and



in which the initial and all final channels with the same n are closely coupled. Note that the resulting set of coupled equations in which exchange is neglected are not the semi-classical analogues or even approximations to the actual coupled differential equations obtained from the full close-coupling method (cf. Burke and Webb, 1970).

In Figs. (1-3) are displayed the total cross sections, labelled FE,

$$\sigma_T(E_i) = 2\pi \frac{k_f}{k_i} \int_0^\pi |f_{if}(\theta, \phi)|^2 \sin \theta \, d\theta \quad (16)$$

computed as a function of electron-impact energy E_i together with various theoretical results and experimental measurements, as referenced in the captions. For process (14), curve EB is an approximation to FE in which $K_n = k_n$ and I_2 in (9) and the term within square brackets in (8) are ignored. For (15), two sets of orthogonal wavefunctions for He ($n = 2$) are used. The cross sections labelled FE1 and FE2 refer to calculations performed with the analytical wavefunctions respectively given by Flannery (1970) and the multi-parameter Hartree-Fock frozen core set of McEachran and Cohen (1969) and of Crothers and McEachran (1970).

The figures provide an indication of the overall ability of the present method, and very little need be said. The situation appears rather encouraging.

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Figure 1: Cross sections for the 2p and 2s excitations of H(1s) by electron impact. Theory: FE, full eikonal treatment; EB, eikonal approximation B ($k_n = k_n$); S, second-order potential method; B, Born approximation; \odot , pseudo-state method; \times , polarized-orbital distorted wave model; \square , four-state impact-parameter method; Experiment: \blacktriangle .

Figure 2: Total cross sections for (a) the 2^1P and (b) the 2^1S excitations of He(1^1S) by electron impact. Theory: FE1: Four channel eikonal treatment with first set of atomic wavefunctions; FE2: Four channel eikonal treatment with set of atomic wavefunctions; S: Second-Order potential method with first set of atomic wavefunctions (Berrington et al. (1973)); B: Born-approximations (Bell et al. 1969). Experiment: (2^1P): \blacktriangle : Donaldson et al. (1972); \square : Jobe and St. John (1967); \times : Moustafa-Moussa (1969); \odot : van Eck and de Jongh (1970); (2^1S): \blacktriangle : Lassetire et al. (1970); \times : Miller et al. (1968); \odot : Vriens et al. (1968).

Figure 3: Total cross sections for (a) the 3^1P and (b) the 3^1S excitations of He(1^1S) by electron impact. Theory: FE: Four channel eikonal treatment with Hartree-Fock frozen core wavefunctions; B: Born approximation (Bell et al. 1969). Experiment: \odot : Donaldson et al. (1972); \blacktriangle : Moustafa Moussa et al. (1969); \times van Eck and de Jongh (1970); \square : St. John et al. (1964).

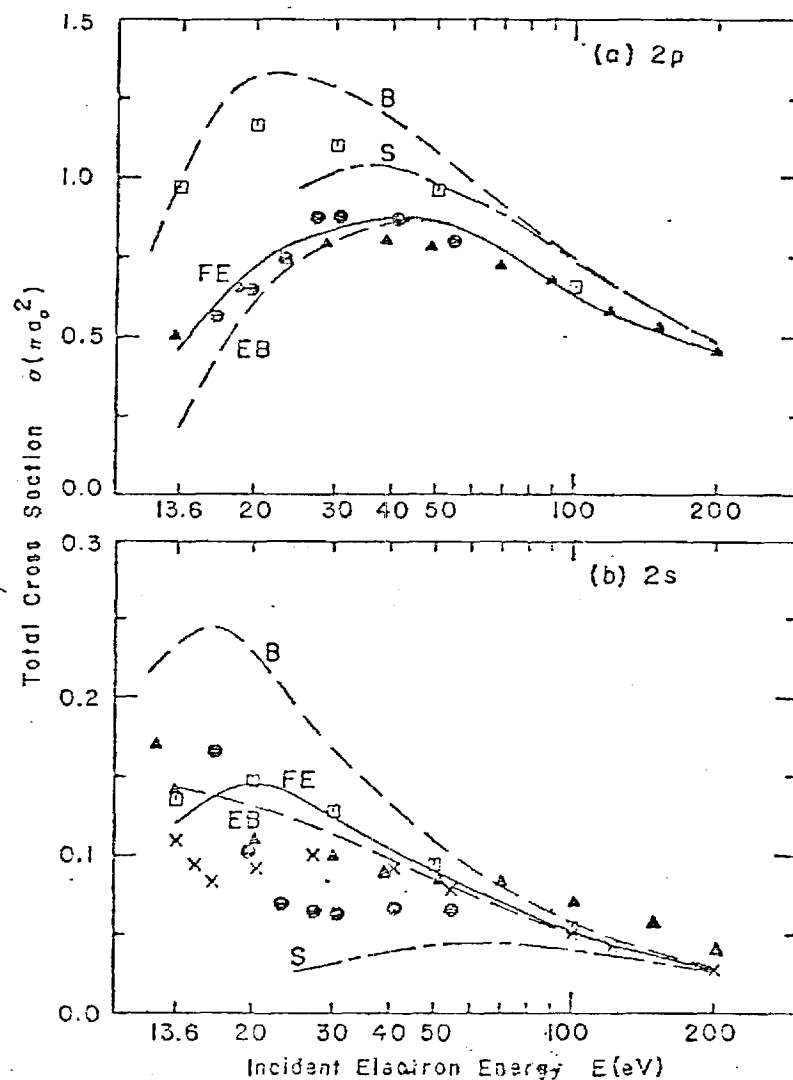


Figure 1: Cross sections for the 2p and 2s excitations of H(1s) by electron impact. Theory: FE, full eikonal treatment; EB, eikonal approximation B ($K_n = k_n$); S, second-order potential method; B, Born approximation; \odot , pseudo-state method; X, polarized-orbital distorted wave model; \square , four-state impact-parameter method; Experiment: Δ .

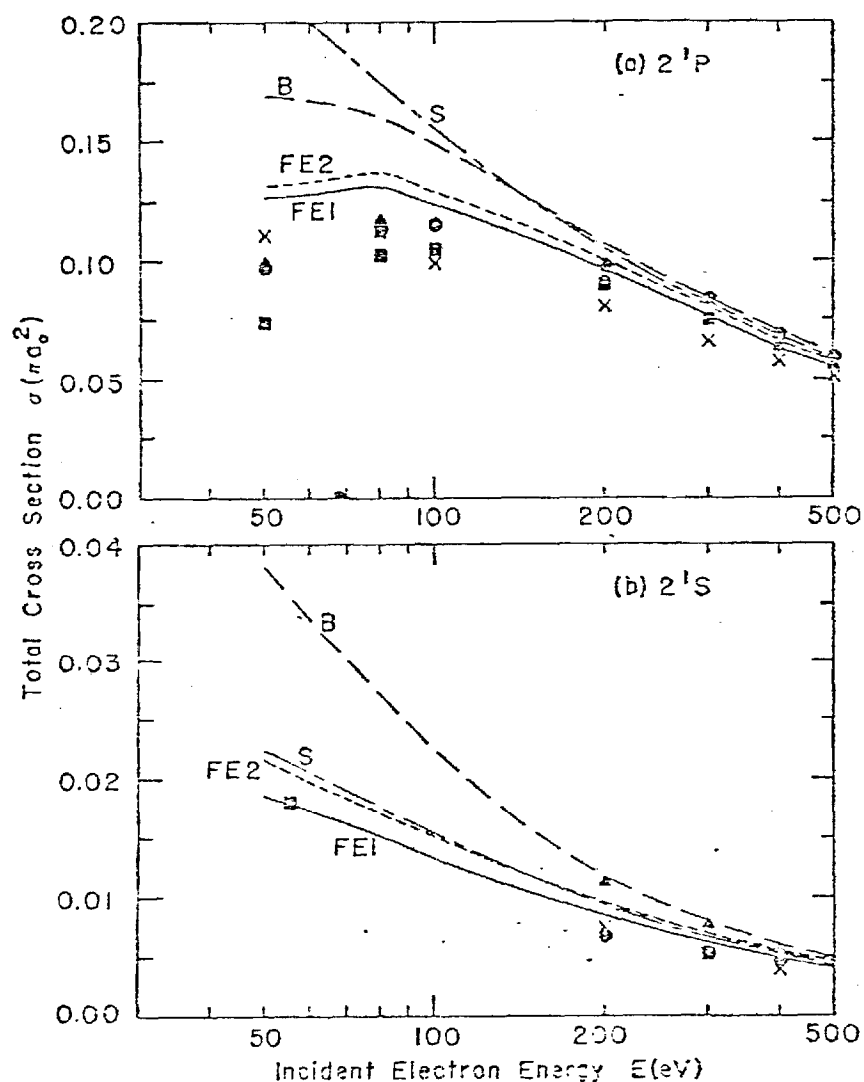


Figure 2: Total cross sections for (a) the 2^1P and (b) the 2^1S excitations of $\text{He}(1^1S)$ by electron impact. Theory: FE1: Four channel eikonal treatment with first set of atomic wavefunctions; FE2: Four channel eikonal treatment with set of atomic wavefunctions; S: Second-Order potential method with first set of atomic wavefunctions (Berrington et al. (1973)); B: Born-approximations (Bell et al. 1969). Experiment: (2^1P): A: Donaldson et al. (1972); B: Jobe and St. John (1967); X: Moustafa-Moussa (1969); O: van Eck and de Jongh (1970); (2^1S): A: Iassetire et al. (1970); X: Miller et al. (1963); O: Vriens et al. (1961).

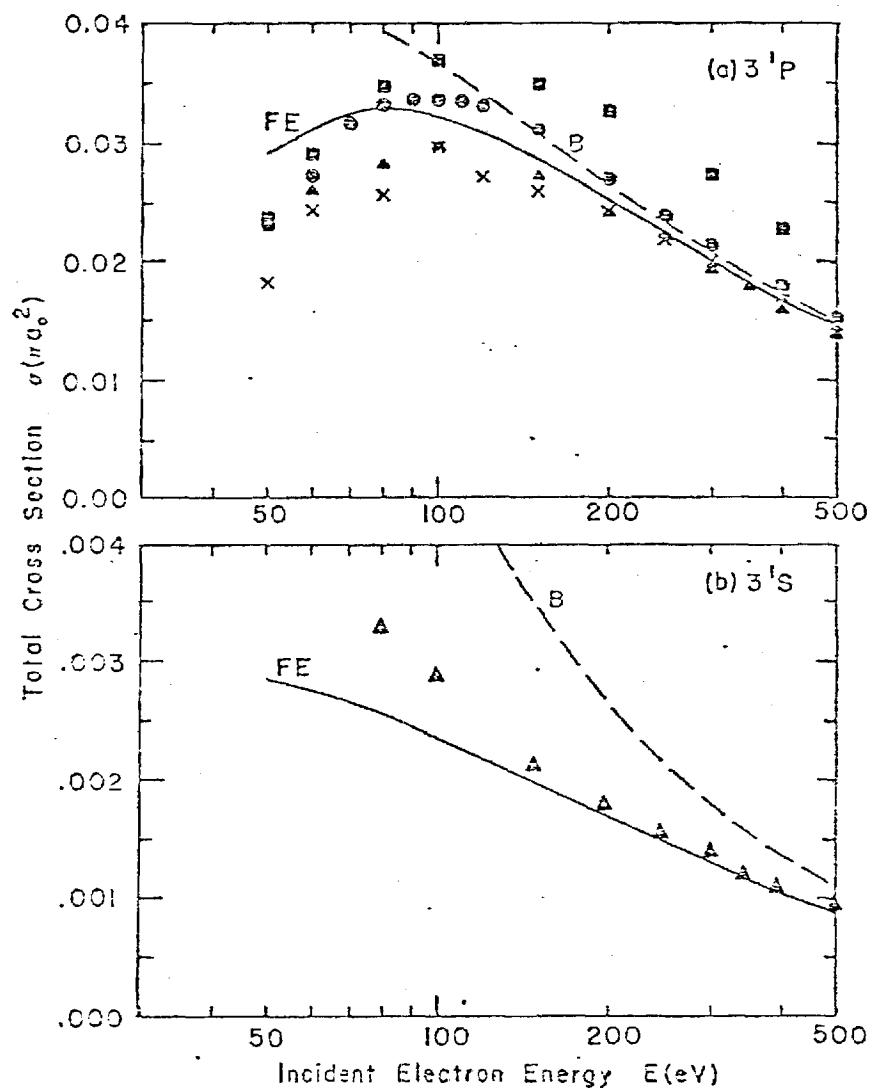


Figure 3: Total cross sections for (a) the $3\ ^1P$ and (b) the $3\ ^1S$ excitations of $\text{He}(1\ ^1S)$ by electron impact. Theory: FE: Four channel eikonal treatment with Hartree-Fock frozen core wavefunctions; B: Born approximation (Bell et al. 1969). Experiment: \circ : Donaldson et al. (1972); Δ : Moustafa Mousa et al. (1969); \times van Eck and de Jongh (1970); \square : St. John et al. (1964).

GEORGIA INSTITUTE OF TECHNOLOGY

ATLANTA, GEORGIA 30332

7 October 1974

SCHOOL OF PHYSICS

Air Force Aerospace Research Laboratories

ATTN: ARL/DO

Contract F33615-74-C-4003

Item No. 0002, Sequence No.

Wright-Patterson AFB, OH 45433

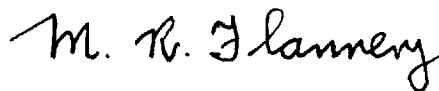
SUBJECT: Quarterly R and D Status Report
Principal Investigator, M. R. Flannery
covering the period 8 July - 8 Oct. 74

Gentlemen:

Transmitted herewith are four (4) copies of the subject report.

Should you have any questions or comments regarding this report,
please contact the principal investigator.

Sincerely,



M. R. Flannery
Professor

MRF:jc
Enclosures

REPORT: Fourth Quarterly R & D Status Report
covering the period July 8, 1974 - Oct. 8, 1974

PROJECT-TITLE: Calculation of Electron Impact Cross Sections
from Metastable States in Atomic and Molecular Gases

PRINCIPAL INVESTIGATOR: M. R. Flannery
School of Physics
Georgia Institute of Technology
Atlanta, Georgia 30332

CONTRACT NO: F33615-74-C-4003

SPONSOR CONTACT PERSON: Lt. John F. Prince / Dr. Alan Garscadden
U. S. Air Force
Air Force Systems Command
Bldg. 450, Area B
Hg. 4950th Test Wing, 4950 (PM MA)
Wright-Patterson, AFB, Ohio 45433

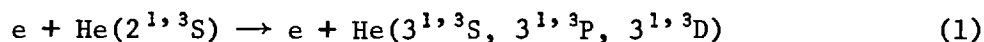
Excitation: (1) In order to complete the present series of tests of the multichannel eikonal approximation, the effect of including the $3\bar{S}$ and $3\bar{P}$ pseudostates is examined for the 2s and 2p excitations of atomic hydrogen by incident electrons with energy E in the range $16.5 \leq E \leq 200$. Very good agreement was obtained with experiment.

A paper describing this work has been written up, is being submitted for publication in J. Phys. B: Atom. molec. Phys. and is included as Appendix A of this report.

(2) Various excitations arising from $e - \text{He}(2^{1,3}S)$ collisions were examined by application of the Born and of the Vainshtein, Presnyakov and Sobel'man approximations. Contrary to expectation, excitation to the $3^{1,3}D$ and $3^{1,3}S$ states dominate the $3^{1,3}P$ and $4^{1,3}P$ excitations at incident energies ≤ 100 eV. A paper describing this work has been written up, will be submitted for publication in J. Appl. Phys.

, and appears as Appendix B of this report.

(3) The multichannel Eikonal Approximation is at present being applied to



Full close-coupling calculations are being performed in which the 1^1S , 2^1S , 3^1S , $3^1P_{0, \pm 1}$ and $3^1D_{0, \pm 1, \pm 2}$ are being closely coupled. As has already been pointed out in Progress Report No. 1, 8 Oct. 73 - 8 Jan. 74, the effect including the 3^1S and 3^1D levels is thought to be significant.

These calculations involve the solution of ten coupled differential equations in which the interaction potentials coupling the various electronic channels need to be accurately determined. One cross section involves ~ 30 mins computer time in U1108 (\equiv CDC 6400).

Publications: (1) The paper entitled "The Multichannel Eikonal Treatment of Atomic Collisions: e - H(1s) elastic and inelastic scattering" was accepted for publication in J. Phys. B: Atom. molec. Phys.

(2) The paper entitled "The Multichannel Eikonal Treatment of Atomic Collisions: The 2^1S and 2^1P inelastic scattering of electrons by helium" has been accepted for publication in the December issue of Physical Review A.

(3) The paper entitled "The Multichannel Eikonal Treatment of Electron-Atom Collisions" has been accepted for publication in "Proceedings of the International Conference on Electron and Photon Interactions with Atoms" (Plenum Press).

Presentations: A paper entitled "The Multichannel Eikonal Treatment of Atomic Collisions" was read by M. R. Flannery at the "The Fourth International Conference on Atomic Physics", 22 - 26 July, 1974.

Degrees Awarded: K. J. McCann was awarded a Ph.D. degree by the Georgia Institute of Technology for a thesis entitled "A Semi-Classical Theory for Differential and Total Scattering Cross Sections with Application to Electron-Atom, Ion-Atom and Atom-Atom Scattering".

Appendix A: To be submitted for
publication as a paper in J. Phys. B:
Atom. molec. Phys.

A Pseudostate Multichannel Eikonal Study of $e - H(1s)$ Inelastic Collisions

M. R. Flannery and K. J. McCann

School of Physics

Georgia Institute of Technology

Atlanta, 30332, U.S.A.

Abstract: The effect of including the $3\bar{s}$ and $3\bar{p}$ pseudostates is examined for the 2s and 2p excitation of atomic hydrogen by incident electrons with energy $E(\text{eV})$ in the range $16.5 \leq E \leq 200$. The 2s - excitation is most strongly affected and displays a behaviour consistent with measurement and refined theories which include polarization. The 2p - excitation agrees particularly well with the full quantal pseudostate treatment and with experiment. A seven channel (1s, 2s, 2p, 3s, 3p) treatment is also performed, and the resulting 2s and 2p cross sections lie closer to those of the pseudostate description than to the four-channel (1s, 2s, 2p) results, as expected.

In this letter, the multichannel eikonal approach (Flannery and McCann, 1975) is examined for the excitations,

$$e + H(1s) \longrightarrow e + H(2s, 2p, 3s, 3p) \quad (1)$$

in which the $3\bar{s}$ and $3\bar{p}$ pseudostates of Burke and Webb (1970) are explicitly acknowledged. In this treatment, the amplitude for scattering with final relative momentum \underline{k}_f in direction (θ, ϕ) with respect to polar axis along the direction of incident relative momentum \underline{k}_i is, in the CM-frame,

$$f_{if}(\theta, \phi) = -i^{\Delta+1} \int_0^\infty J_\Delta(K'\rho) [I_1(\rho, \theta) - i I_2(\rho, \theta)] \rho d\rho \quad (2)$$

where J_Δ are Bessel functions of integral order, and where K' is the XY-component $k_f \sin \theta$ of the momentum-change $\underline{K} = \underline{k}_i - \underline{k}_f$. The collision functions

$$I_1(\rho, \theta; \alpha) = \int_{-\infty}^\infty \kappa_f(\rho, Z) \left[\frac{\partial C_f(\rho, Z)}{\partial Z} \right] \exp(i\alpha Z) dZ \quad (3)$$

and

$$I_2(\rho, \theta; \alpha) = \int_{-\infty}^\infty \left[\kappa_f(\kappa_f - k_f) + \frac{\mu}{\hbar^2} V_{ff} \right] C_f(\rho, Z) \exp(i\alpha Z) dZ \quad (4)$$

contain a dependence on the scattering angle θ via

$$\alpha = k_f(1 - \cos \theta) = 2k_f \sin^2 \frac{\theta}{2} \quad (5)$$

the difference between the Z-component of the momentum change \underline{K} and the minimum change $k_i - k_f$ in the collision. The coupling amplitudes C_f are solutions of the following set of N-coupled linear equations

$$\frac{i\hbar^2}{\mu} \kappa_f(\rho, Z) \frac{\partial C_f(\rho, Z)}{\partial Z} + \left[\frac{\hbar^2}{\mu} \kappa_f(\kappa_f - k_f) + V_{ff}(\rho, Z) \right] C_f(\rho, Z) =$$

$$\sum_{n=1}^N C_n(\rho, Z) V_{fn}(\rho, Z) \exp i(k_n - k_f) Z, f = 1, 2, \dots, N \quad (6)$$

solved subject to the boundary condition $C_f(\rho, \infty) = \delta_{if}$. The local wavenumber of relative motion at separation $\underline{R} \equiv (R, \Theta, \Phi) \equiv (\rho, \Phi, Z)$ is

$$K_n(\underline{R}) = [k_n^2 - \frac{2\mu}{\hbar^2} V_{nn}(\underline{R})]^{1/2} \text{ where the interaction matrix elements}$$

$V_{nm}(\underline{R}) = \langle \phi_n(\underline{r}) | V(\underline{r}, \underline{R}) | \phi_m(\underline{r}) \rangle$ connect the various electronic states $\phi_n(\underline{r})$ describing the isolated systems and where $V(\underline{r}, \underline{R})$ is the instantaneous electrostatic interaction.

The present description has automatically included an infinite number of partial waves of relative motion which are distorted by the static interactions associated with the various channels included in the basis set expansion and which in turn are coupled to the internal electronic motions via the amplitudes C_f in (6). Moreover in contrast to previous semiclassical descriptions* explicit account is taken of the variation during the collision of the different local momenta of relative motion in each channel.

Close-coupling calculations have been performed by using (2) - (6) in which the 1s, 2s, $2p_{0,\pm 1}$ states of atomic hydrogen are included together (a) with the $3\bar{s}$ and $3\bar{p}$ pseudostates of Burke and Webb (1970) introduced to acknowledge couplings to all higher open channels and (b) with the actual 3s and 3p atomic states. In tables 1 and 2 are displayed total excitation cross sections.

$$\sigma_f(E) = 2\pi \frac{k_f}{k_i} \int |f_{if}(\theta, \phi)|^2 d(\cos \theta) \quad (7)$$

for processes (1) at incident electron-energy $E(\text{eV})$. Previous four-channel results F for the 2s and 2p excitations (Flannery and McCann, 1975) converge from above and below respectively onto the pure seven-channel treatment R.

* cf. Flannery and McCann (1974) when $I_2 = 0$, $K_f = k_f$ in (3) and (6) and coefficient of C_f in LHS of (6) neglected, and cf. Bransden (1970).

Addition of the pseudostates in P considerably distorts the shape and changes the magnitude of the 2s-excitation while σ_{2p} remains relatively unaffected. Replacing the pseudostates by the real 3s and 3p states in general yields cross sections which lie between F and P although closer to P, as expected.

These effects are further illustrated in figs. 1 and 2 where comparison theoretical and experimental data are provided. In fig. 1a, the 2p-measurements of Long et al. (1968) are normalized to the present F value at 200 eV (rather than to the Born cross section which is 7% higher). The recent absolute measurement of Williams and Willis (1974) at 11 eV is 13% higher than the corresponding 2p-cross section of Long et al. The present σ_{2p} are in very good agreement with the experiment and with the fully quantal pseudostate treatment of Burke and Webb. The recent twenty-state second-order diagonalization impact-parameter description of Baye and Heenan (1974) for the 2p and 3p excitations, in fig. 1, is in close accord with the second-order potential treatment of Bransden et al. (1972) and Sullivan et al. (1972), an approach based on the impact-parameter method, and designed to acknowledge couplings with all excited states. Born and Glauber (cf. Tai et al., 1970) cross sections are also included in the figures.

In fig. 2, the main effect of pseudostate-addition causes the 2s-cross section to continue its increase as the impact-energy E is reduced to 16.5 eV, reflecting a behaviour also exhibited by the treatments of Burke and Webb, and of McDowell et al. (1973). This behaviour is real and is consistent with the measurements shown in fig. 2b of Kauppila et al. (1970) who estimate a cascade contribution of $0.23 \sigma_{3p}$ to the observed 2s-excitation. The present 3s-cross sections are shown in fig. 3 together with other theoretical values, for comparison.

Rather than presenting all the differential cross sections, from which σ_f in (7) were obtained, it suffices to report that the 2p-scattering did not depart

appreciably from the earlier study (Flannery and McCann, 1975). In fig. 4, the pseudostates reduce the 2s-scattering at 100 eV in the forward direction and enhance the scattering through larger angles, the net result being a slight increase in the total cross section at 100 eV. This behaviour becomes increasingly amplified as the impact-energy E is reduced and figures similar to (4) are available upon request.

In contrast, pseudostates increase the four-channel elastic scattering in the forward direction as expected since the potential appropriate to the distant elastic encounters becomes more long-range. Hence, agreement with the experiment of Teubner et al. (1973) became somewhat improved for small-angle scattering. However, because of the neglect of electron-exchange needed for a proper description of closer encounters, the present treatment still failed (Flannery and McCann, 1975) to provide a good description (cf. Winters et al., 1974) of elastic scattering through the larger scattering angles.

In conclusion, addition of pseudostates does improve the agreement for inelastic collisions of the present multichannel eikonal approach with experiment and with other refined theories which include polarization effects. In particular, the continuing rise of σ_{2s} as E is reduced to below ~20 eV is consistent with experiment (cf. fig. 2b), although, at these low energies, electron-exchange is important and could cause the required reduction needed to improve accord between the present approach and experiment (cf. fig. 2b).

Acknowledgment: This research was sponsored by the Air Force Aerospace Research Laboratories, Air Force Systems Command, United States Air Force, Contract F 33615-74-C-4003.

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B: Atom. molec. Phys. 7, 788-98.

Table I

Total cross sections (πa_0^2) given by a four-channel treatment F, and two seven-channel treatments (P and R, with and without pseudostates, respectively) of $e + H(1s) \rightarrow e + H(2s \text{ or } 2p)$ at electron-energy E (eV).

E nℓ	2s			2p ₀	2p _{±1}	2p		
	F	P	R	P	P	F	P	R
16.5	-	0.151	0.112	0.405	0.125	-	0.530	0.600
20	0.145	0.127	0.124	0.481	0.224	0.720	0.705	0.730
30	0.124	0.095	0.115	0.485	0.379	0.836	0.864	0.863
50	0.090	0.074	0.088	0.421	0.466	0.865	0.887	0.881
100	0.052	0.048	0.052	0.227	0.421	0.629	0.648	0.645
200	0.028	0.027	0.028	0.120	0.338	0.453	0.458	0.454

Table II

Total cross sections ($0.01 \pi a_0^2$) given by seven-channel treatment
of $e + H(1s) \rightarrow e + H(nl)$; $nl = 3s, 3p_0, 3p_{\pm 1}$, at electron-energy
E (eV)

$\begin{array}{c} nl \\ E \end{array}$	3s	$3p_0$	$3p_{\pm 1}$	3p
16.5	1.41	5.04	2.19	7.23
20	1.78	6.67	4.23	10.9
30	1.87	7.25	7.52	14.8
50	1.46	5.65	8.96	14.6
100	0.90	3.13	8.00	11.1
200	0.50	1.61	5.81	7.42

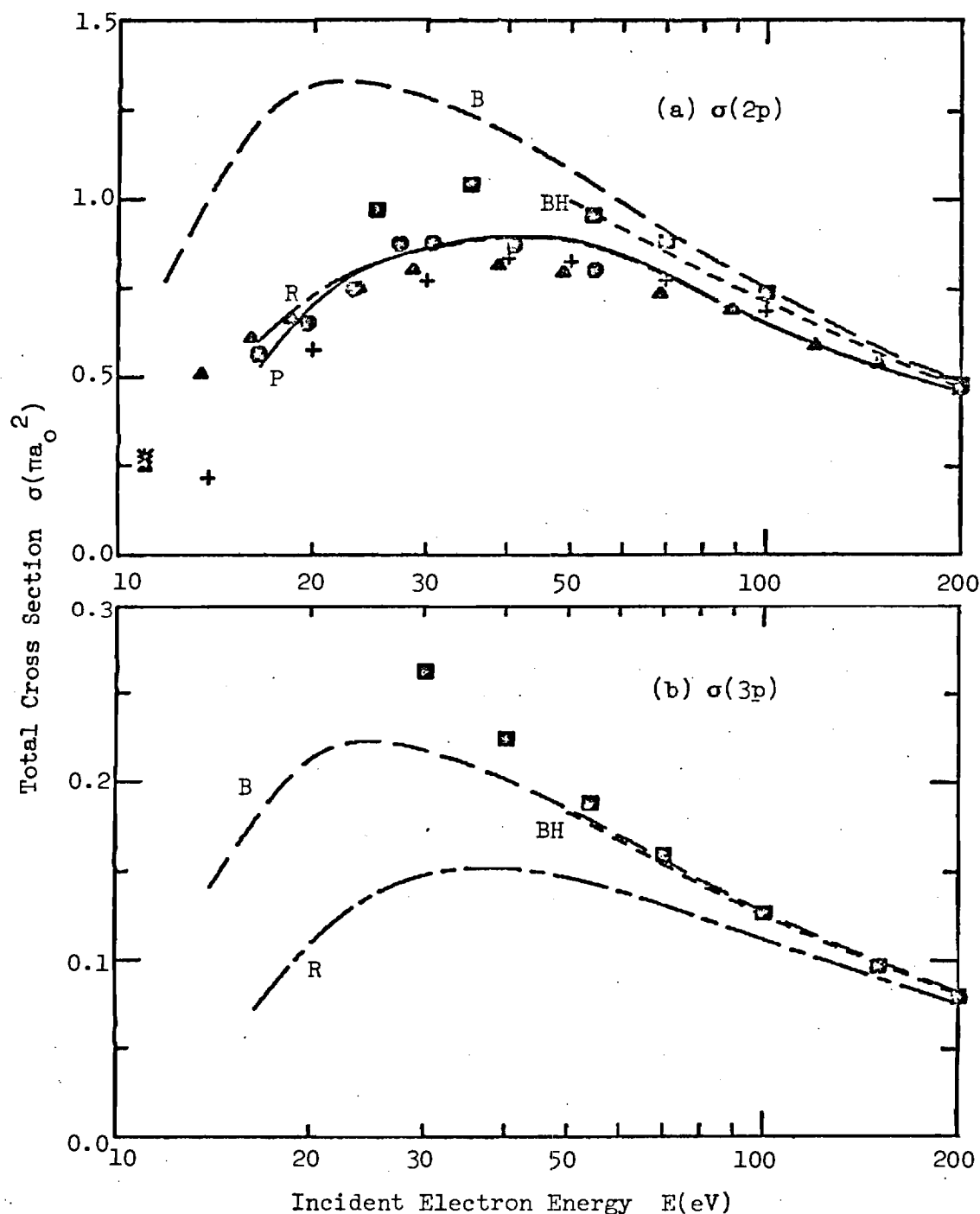


Figure 1. Cross sections (πa_0^2) for (a) the 2p and (b) the 3p excitations from H(1s) by electrons with energy E (eV). P and R are the present seven-channel results with pseudo and real 3s and 3p states respectively. Experiment: Δ (Long et al. 1968), \times (Williams and Willis, 1974), theory: pseudo-state (Burke and Webb, 1970), second-order potential method: (a) four-channel approximation (Sullivan et al. 1972), (b) one-channel approximation (Bransden et al. 1972), + Glauber approximation (Tai et al. 1970), BH Baye and Heenan (1974), B Born approximation.

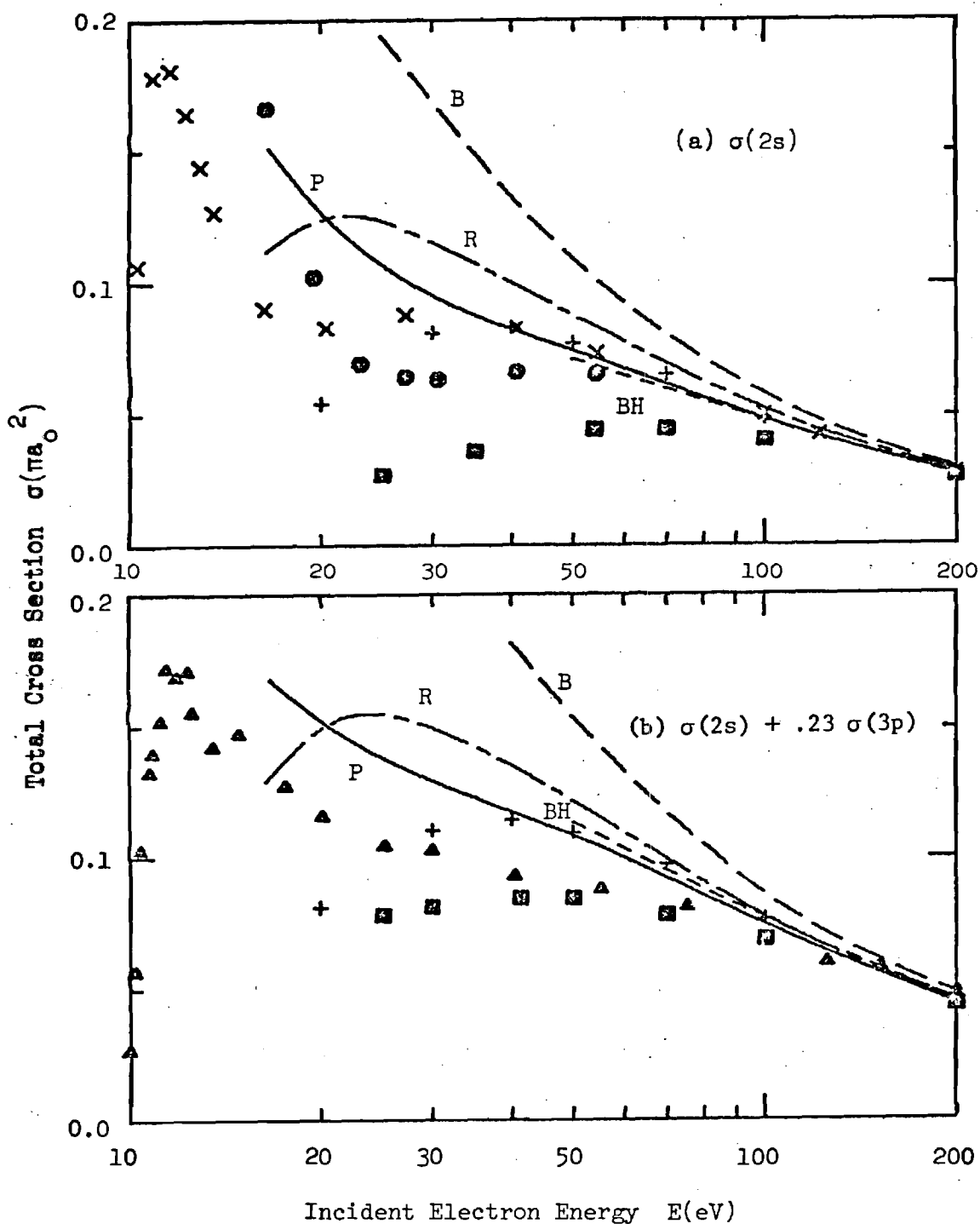


Figure 2. Cross sections for the 2s-excitation from H(1s) by electrons with energy E (eV). Notations as in figure 1, except experiment: Δ (Kauppila et al. 1970), theory: X McDowell et al. (1973).

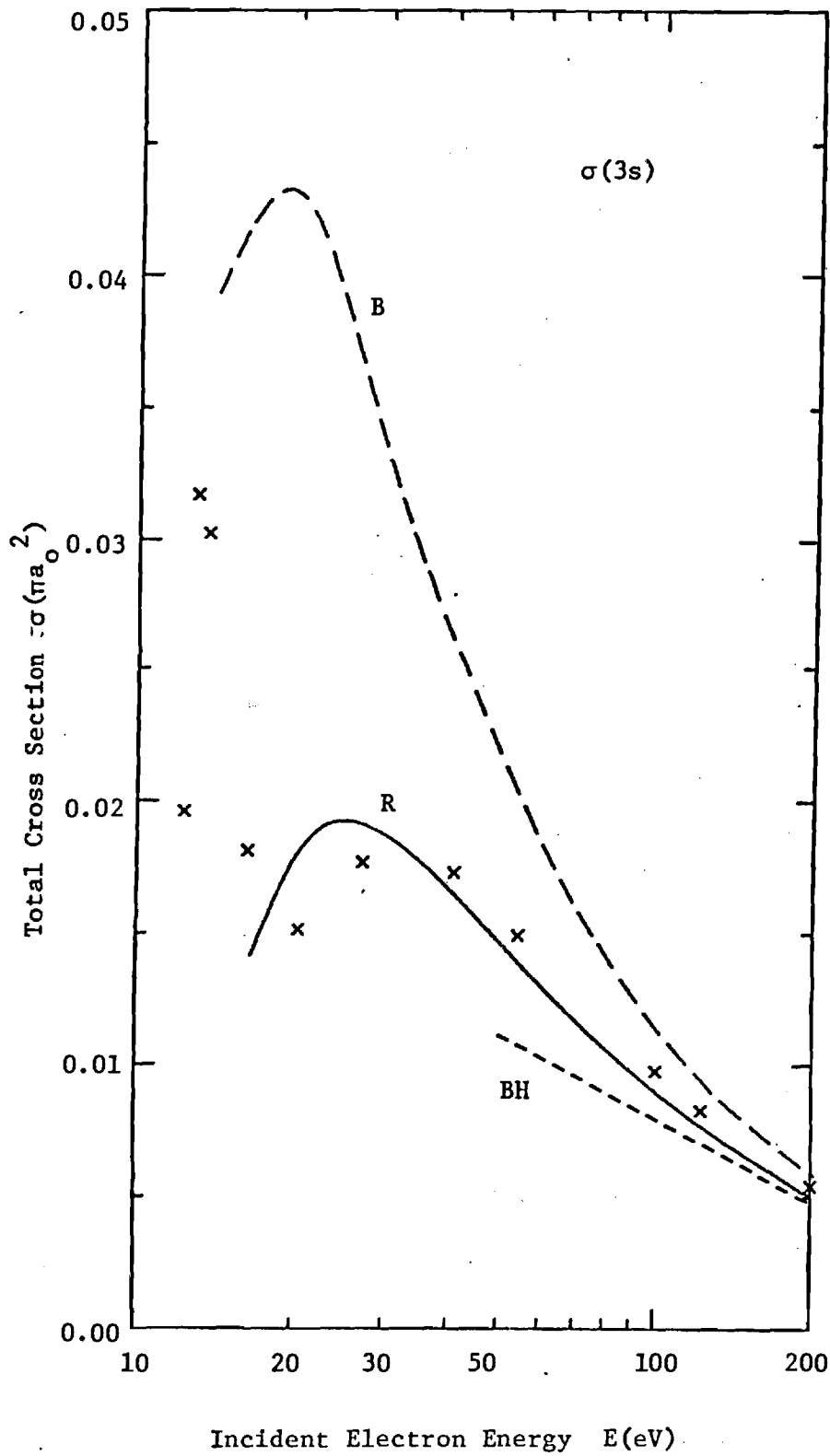


Figure 3. Cross sections (πa_0^2) for the 3s-excitation from H(1s) by electrons with energy $E(\text{eV})$. Notation as in figure-2.

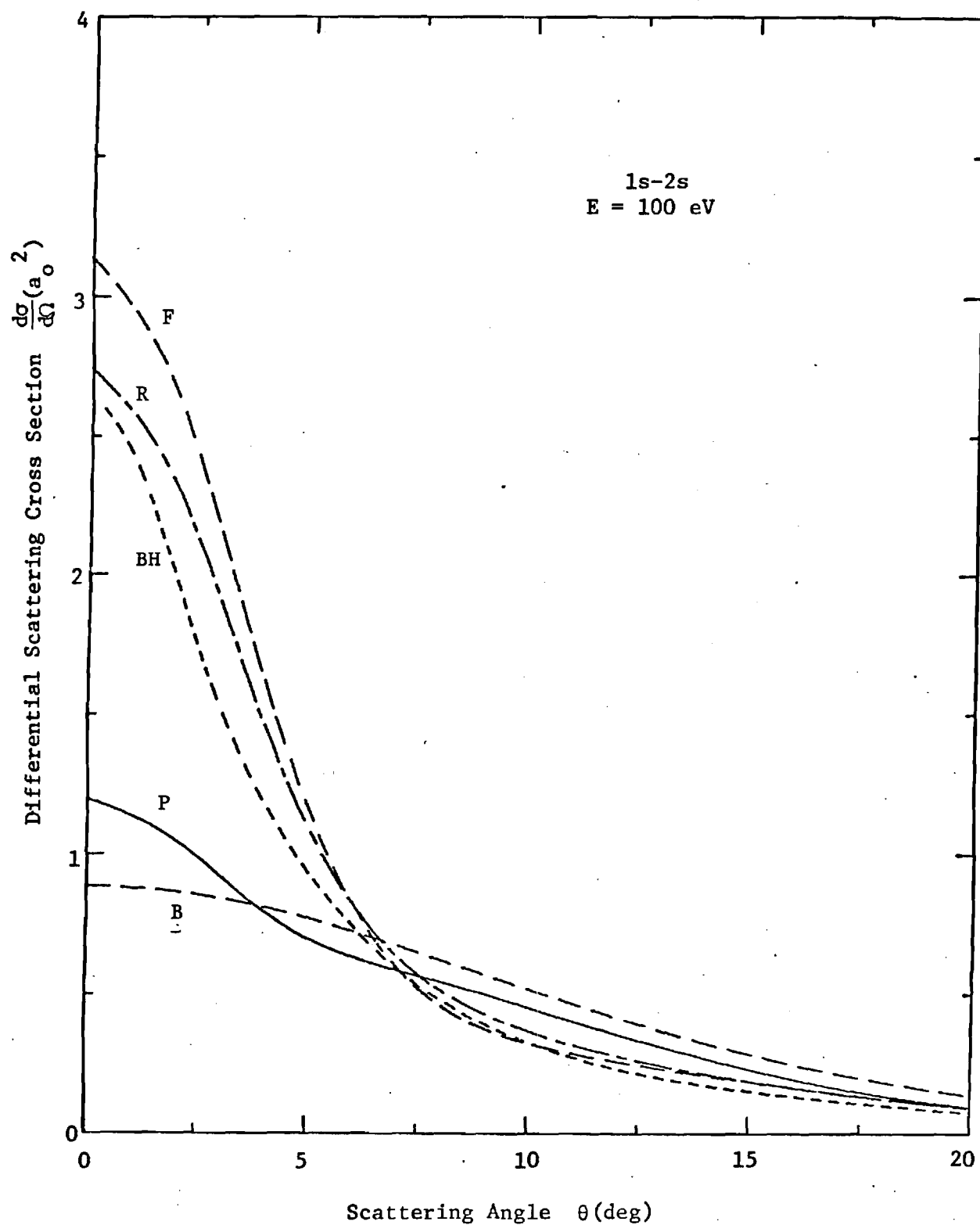


Figure 4. Differential cross sections for 2s-excitation from H(1s) at 100 eV impact-energy. Notation as in figure 1 with F: four-channel treatment (Flannery and McCann 1975)

Appendix B: To be submitted for
publication as a paper in J. Applied Phys.

Excitation in Electron-Metastable Helium Collisions*

M. R. Flannery, W. F. Morrison and B. L. Richmond

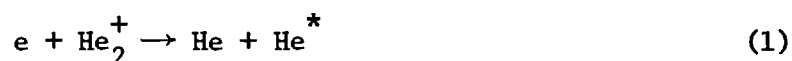
School of Physics
Georgia Institute of Technology
Atlanta, Georgia 30332

Abstract

The $2^{1,3}P$, $3^{1,3}S$, $3^{1,3}P$, $3^{1,3}D$ and $4^{1,3}P$ excitations arising from $e - He(2^{1,3}S)$ collisions are examined by application of the Born and of the Vainshtein, Presnyakov and Sobel'man approximations. Total excitation cross sections are calculated for the above transitions for electron impact-energy E up to 500eV. Contrary to expectation, excitation to the $3^{1,3}D$ and $3^{1,3}S$ states dominate the $3^{1,3}P$ and $4^{1,3}P$ excitations except at incident energies above 100eV.

I. Introduction

While theoretical and experimental knowledge of collisions between electrons and ground-state atomic species has increased significantly during the past decade, relatively little¹ is known with any great certainty about collisions involving metastables. In a high-density gas discharge, metastable states are populated predominantly by dissociative recombination



between slow electrons and molecular ions formed initially by the rapid three-body association process



In (1), the excited levels with principal quantum number $n \geq 3$ (except, perhaps, the $3^1,^3\text{S}$ states) are depleted by dissociative ionization (or the Hornbeck-Molnar process)

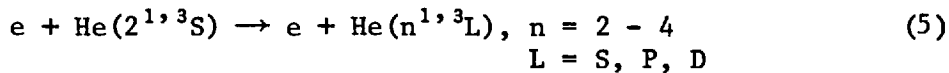


thereby ensuring that the $2^1,^3\text{S}$ metastable states, which are also formed by direct electron-impact excitation from the ground state, are the dominant excited atomic species. The rates of the subsequent collision processes involving the metastables are very important to the analysis of gaseous discharges and gaseous nebulas² and are at present unknown. In vacuum UV-lasers, for example, excited molecular states He_2^* are formed mainly by



which radiate photons of wavelength $\sim 610\text{\AA}$ to the dissociative ground state, thereby

ensuring automatic population inversion. The metastable content He^* formed via (1) is primarily depleted by the excitation processes,



the cross sections for which would critically affect the overall formation rate of He_2^* by (4). Any information on the above processes (5) is very scarce.

In an effort to systematically explore the various processes involving metastables, we will consider in this paper the excitation cross sections for (5) by using initially the simpler theoretical approaches - the Born¹ and the Vainshtein, Presnyakov and Sobel'man (VPS) approximations³. Various effects such as the repulsion between the incident and excited electrons, effective-charge and electron-exchange effects are included to first order in the VPS method. Not only will this present investigation establish some remarkable properties of the cross sections but also will provide the additional insight to the collision needed as a basis for more refined descriptions.

II. Theory

According to the Born approximation¹ for electron-atom collisions, the total cross section for excitation of state n from an initial state i of the target atom is given by

$$Q_{in}(k_i) = \frac{8\pi}{k_i^2 a_0^2} \int_{k_i - k_n}^{k_i + k_n} |F_{in}(K)|^2 \frac{dK}{K^3} \quad (6)$$

in atomic units (a_0^2) where

$$F_{in}(K) = \langle \phi_i(r_1, r_2) | \sum_{j=1}^2 \exp(i\mathbf{K} \cdot \mathbf{r}_j) | \phi_n(r_1, r_2) \rangle \quad (7)$$

is generalized form factor connecting states i and n of atomic helium, the bound

electrons at \mathbf{r}_1 and \mathbf{r}_2 being described by the set of wavefunctions $\phi_n(\mathbf{r}_1, \mathbf{r}_2)$ with eigenenergies ϵ_n . The vector $\mathbf{K} = \mathbf{k}_1 - \mathbf{k}_n$, where \mathbf{k}_1 and \mathbf{k}_n are the initial and final wavenumbers of relative motion, is the momentum-change suffered by the collision. From a knowledge of the form factor (7), the excitation cross sections are easily calculated from (6).

In Born's approximation, however, and in more refined descriptions, e. g. the close coupling method, the total wavefunction for the collision system is expanded in terms of unperturbed atomic states, the interaction between the incoming electron and the atom being treated as a perturbation, assumed small. In this instance, the averaged attraction of the incident electron with the screened nucleus is of primary importance while details of repulsion with the atomic electrons is ignored in the wavefunction describing the relative motion. However, when an atom is initially in an excited state, the electron is generally quite distant from the core (for H(n), $r_1 = n^2 a_0$; for He(2^1S) $r_{12} = 5.3 a_0$) and hence, the incident electron is subjected, not to the averaged field of the orbital electron about the core but actually to two strong Coulomb fields - the e - e repulsion and the e - core attraction. These two fields reduce to the averaged field only for distant encounters.

For electron-hydrogen scattering, Vainshtein et al.³ have introduced a method whereby a product of Coulombic functions is chosen to represent the zero-order (unperturbed) wavefunction for the e - H relative motion. The method achieved notable success for e - H(1s) excitation and ionization. The extension of their analysis to e - He($2^1, ^3S$) collisions is straightforward, and results in the cross section,

$$Q_{in} = \frac{8\pi}{k_1^2 a_0^2} \int_{k_1 - k_n}^{k_1 + k_f} |F_{in}(\mathbf{K})|^2 [f(v, x)]^2 \frac{dK}{K^3} \quad (8)$$

in which the integrand of (6) is multiplied by the square of the factor,

$$f(v, x) = \left[\frac{\pi v}{\sinh \pi v} \right] F(-iv, iv, 1, x) \quad (9)$$

where F is a hypergeometric function with arguments,

$$x = \left[\frac{2 \epsilon_{ni} + K^2}{2 \epsilon_{ni} + 3K^2} \right], \quad v = k_i^{-1} \quad \text{or} \quad (k_i + \sqrt{2\epsilon_i})^{-1} \quad (10)$$

in which $\epsilon_{ni} = \epsilon_n - \epsilon_i$ is the excitation energy in atomic units (27.2 eV) and where the second value of v in (6) is designed to account for the fact that the atomic electrons are bound so as to give an effective-charge effect.

The effect of exchange between the incident and atomic electrons is ignored by (6) and (8). Its acknowledgement involves explicit inclusion of spin functions. For singlet-singlet transitions the overall spin state for the (e - He) system is a doublet and the total wavefunction for the three-electrons denoted by 1, 2, and 3 is, in a two-state treatment, given by,

$$\begin{aligned} \Psi^S(1, 2; 3) &= \frac{N_S}{\sqrt{3}} \sum_{\text{cyclic } 1,2,3} \left[\Psi_i^S(1, 2) F_i(3) + \Psi_n^S(1, 2) F_n(3) \right] \chi^-(1, 2; 3) \\ &\equiv \Psi_i + \Psi_n \end{aligned} \quad (11)$$

where $F_n(3)$ is the wavefunction describing the projectile-target relative motion, where

$$\chi^-(1, 2; 3) = \frac{1}{\sqrt{2}} (\alpha_1 \beta_2 - \beta_1 \alpha_2) \alpha_3 \quad (12)$$

is the normalized doublet spin function, and where $\Psi_n^S(1, 2) = \Psi_n^S(2, 1)$ is the symmetrical spatial wavefunction for singlet helium. The overall wavefunction Ψ^S , normalized by N_S , is antisymmetric with respect to interchange of any two electrons. The Born approximation to the amplitude for scattering by angle θ , is therefore,

$$F_{in}(\theta) = - \frac{1}{4\pi} \frac{2me^2}{\hbar} \sum_{m_{s_1}} \sum_{m_{s_2}} \sum_{m_{s_3}} \langle \psi_n | V | \psi_i \rangle_{\underline{r}_1, \underline{r}_2, \underline{r}_3} \quad (13)$$

where $V(\underline{r}_1, \underline{r}_2, \underline{r}_3)$ is the e - He electrostatic interaction and $F_i(3) = \exp(i\mathbf{k}_i \cdot \underline{r})$.

On performing the cyclic summations in (11), on summing over the spin substates $m_s = \pm \frac{1}{2}$ in (13) and on using the orthonormal properties of the spin functions α_i and β_i , then, the scattering amplitude reduces, after some analysis, to

$$F_{in}^{SS}(\theta) = N_S^2 [f_{in} - g_{in}] \quad (14)$$

where

$$f_{in}(\theta) = - \frac{1}{4\pi} \frac{2me^2}{\hbar} \langle \psi_n^S(1, 2) F_n(3) | V | \psi_i^S(1, 2) F_i(3) \rangle \quad (15)$$

is the scattering amplitude for direct collisions alone and

$$g_{in}(\theta) = - \frac{1}{4\pi} \frac{2me^2}{\hbar} \langle \psi_n^S(3, 2) F_n(1) | V | \psi_i^S(1, 2) F_i(3) \rangle \quad (16)$$

represents the scattering amplitude for exchange collisions in which electrons 1 and 3 have been interchanged. By taking $F_{i,n}$ to be a plane waves, then (14) - (16) gives rise to the Born-Oppenheimer approximation¹. By taking F_n to be a plane wave and F_i to be a product of unperturbed Coulombic waves, then the following expression

$$g_{in}^{VPS} = \frac{K^2}{2k_i^2} f\left(\nu, \frac{1}{4}\right) f_{in}^B \quad (17)$$

for the exchange amplitude can eventually be derived from application of the VPS approximation which also assumes $\langle \psi_i | \psi_n \rangle = \delta_{in}$ and hence $N_S = 1$ in (14). Then, the total cross section including exchange for singlet-singlet transitions is finally,

$$Q_{in}^{1,1}(k_i) = \frac{2\pi k_n}{k_i} \int \left| F_{in}^{SS}(\theta) \right|^2 d(\cos \theta) = \frac{8\pi}{k_i^2 a_o^2} \int_{k_i - k_n}^{k_i + k_n} \frac{|F_{in}(K)|^2}{K^3} \left[f(\nu, x) - \frac{K}{2k_i^2} f\left(\nu, \frac{1}{4}\right) \right]^2 dK \quad (18)$$

For the triplet-triplet transitions in (5), the overall antisymmetric spatial-spin statefunction can either belong to a doublet or as a quartet spin state. Scattering in the doublet mode occurs in $\frac{1}{3}$ of all collisions while $\frac{2}{3}$ of all collisions are in a quartet mode. The total wavefunction analogous to (11) is therefore,

$$\begin{aligned}\Psi^T(1, 2; 3) &= \frac{N_T}{\sqrt{3}} \sum_{1,2,3}^{\text{cyclic}} [\Psi_i^A(1, 2) F_i(3) + \Psi_n^A(1, 2) F_n(3)] \chi_{Q,D}^+(1, 2; 3) \\ &\equiv \Psi_i + \Psi_n\end{aligned}\quad (19)$$

in which $\Psi_i^A(1, 2)$ is the antisymmetric spatial wavefunction for triplet helium and where the three-electron normalized spin functions are

$$\chi_Q^+(1, 2; 3) = \begin{cases} \alpha_1\alpha_2\alpha_3, & M_S = +\frac{3}{2} \\ \frac{1}{\sqrt{3}}(\alpha_1\alpha_2\beta_3 + \alpha_1\beta_2\alpha_3 + \beta_1\alpha_2\alpha_3), & M_S = +\frac{1}{2} \end{cases} \quad (20a)$$

for the quartet spin state with total magnetic components $M_S = \frac{3}{2}$ and $\frac{1}{2}$, and

$$\chi_D^+(1, 2; 3) = \frac{1}{\sqrt{6}} [2\alpha_1\alpha_2\beta_3 - \alpha_3(\alpha_1\beta_2 + \alpha_2\beta_1)], \quad M_S = +\frac{1}{2} \quad (20b)$$

represents the doublet state. The functions appropriate to states with negative magnetic quantum numbers are obtained from (12) and (20) by the $\alpha_i \leftrightarrow \beta_i$ interchange for each of the three electrons in the corresponding function for positive M_S .

By substituting (19) - (20) in (13) and by performing the cyclic summations and the spin summations, then after lengthy, although straightforward, analysis, the following expressions

$$F_{in}^{TT}(D) = N_T [f_{in} + g_{in}] \quad (21a)$$

and

$$F_{in}^{TT}(Q) = N_T [f_{in} - 2g_{in}] \quad (21b)$$

are obtained for the scattering amplitudes in the doublet (D) and quartet (Q) modes, respectively. Since $\frac{1}{3}$ and $\frac{2}{3}$ of all collisions are in the D and Q modes respectively then

$$\left| F_{in}^{TT}(\theta) \right|^2 = \frac{1}{3} \left| F_{in}^{TT}(D) \right|^2 + \frac{2}{3} \left| F_{in}^{TT}(Q) \right|^2 \quad (22a)$$

$$= |f_{in}|^2 - 2\text{Re}(f_{in} g_{in}^*) + 3|g_{in}|^2 \quad (22b)$$

Hence, the total excitation cross section for triplet-triplet transitions is then,

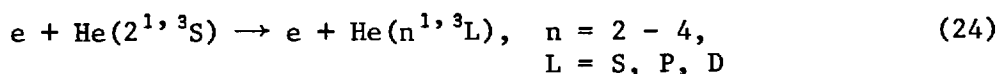
$$Q_{in}^{3,3}(k_i) = 2\pi \frac{k_n}{k_i} \int \left| F_{in}^{TT}(\theta) \right|^2 d(\cos \theta) \quad (23a)$$

$$= \frac{8\pi}{k_i^2 a_0^2} \int \frac{\left| F_{in}(K) \right|^2}{K^3} \left\{ \left[f(v, x) \right]^2 - \frac{K^2}{k_i^2} f(v, \frac{1}{4}) f(v, x) + \frac{3}{4} \frac{K^4}{k_i^4} \left[f(v, \frac{1}{4}) \right]^2 \right\} dK \quad (23b)$$

on application of the VPS approximations (8) and (17) for f_{in} and g_{in} respectively. Note that at high impact-energies, the function $f(v, x) \rightarrow 1$ so that the Born and the Ochkur⁴ approximations are recovered for the direct and exchange scattering amplitudes, respectively. The Ochkur method is a simplification to the original Born-Oppenheimer approximation mentioned above, and is therefore based on the use of plane waves for the relative motion.

III Results and Discussion

The theory outlined above has been applied to the examination of the excitation processes,



for incident-electron energies E from threshold up to 500eV. Highly accurate

form factors (3) have already been computed by Kim and Inokuti⁵ from the extremely reliable correlated wavefunctions of Weiss⁶. The following four sets of cross-section calculations were performed for each transition in (24) - the Born approximation B given by eq. (6), and the three VPS approximations given by eqns. (8 - 10), with and without the effective-charge, and by (18) and (23) which include the additional effect of electron-exchange in singlet-singlet and triplet-triplet transitions respectively.

In figs. (1 - 4) are presented the Born and VPS cross sections (in $\pi a_0^2 = 0.88 \cdot 10^{-16} \text{ cm}^2$) calculated to within 1% accuracy as a function of impact-energy E(eV). The present Born values agree with those previously given by Kim and Inokuti⁵ for the $2^1S - 2^1P$ and the triplet-triplet transitions. The optical linestrengths S for the $2^{1,3}S - 2^{1,3}P$ transition are the largest ($= 25.5$, and 57.7 atomic units respectively⁷) and hence it is only to be expected that the collision cross sections for these excitations dominate. However, fig. 3 demonstrates a remarkable feature at low E when the collisional excitations are in the following descending order $3^1D > 3^1S > 3^1P > 4^1P$. At high E $> 100\text{eV}$, the natural order $3^1P > 3^1D > 3^1S > 4^1P$ is followed when the cross sections $\sim E^{-1} \ln E$ for the optically allowed transitions, and $\sim E^{-1}$ for the optically forbidden transitions. For the singlet transitions $\sigma(3^1S) > \sigma(3^1P)$ from threshold up to $\sim 12\text{eV}$ while $\sigma(3^1D)$ remains greater than $\sigma(3^1P)$ up to 100eV . Fig. 4 demonstrates that similar behavior occurs also for the triplet-transitions the cross over point for the cross sections being shifted however to higher energies i. e. $\sigma(3^3S) > \sigma(3^3P)$ for $E < 100\text{eV}$ and $\sigma(3^3D) > \sigma(3^3P)$ for $E < 1000\text{eV}$.

The basic reason for this unexpected behavior is that the linestrength for the $2^{1,3}S - 3^{1,3}P$ transitions in helium is abnormally small i. e. 2.5 atomic units⁷ to be compared with the value⁷ 18.8 for the $2s - 3p$ transition in atomic hydrogen. The importance of the quadrupole and higher-order optically-forbidden

multipole terms relative to the optically-allowed dipole term is therefore strong such that the optically-forbidden collisional excitations dominate the optically-allowed excitation at low and intermediate impact energies.

The effects acknowledged by the various VPS approximations are demonstrated in fig. 1 for the 2^1P and the 3^1S excitations which were found to be representatives of the optically allowed and forbidden transitions in (24). The use, as in (8) with $v = k^{-1}$, of the zero-order Coulombic functions for the relative motion (instead of a plane wave) yields, in general, cross sections which are lower than the Born values in the low and intermediate energy region and which eventually converge onto the correct Born limit at high energies. The optically allowed transitions are affected more by this inclusion than are the optically forbidden excitations. When the effective-charge is acknowledged by the use of $v = (k_i + \sqrt{2\epsilon_i})^{-1}$ in (8) - (9), all the cross sections are significantly increased. The additional inclusion of exchange, as by (18) and (23), causes a relatively smaller decrease. The use of more refined wavefunctions for the relative motion thus appears to be more important than the inclusion of exchange.

This claim is further supported in fig. 2 by the close-coupling study of Burke et al.⁸ who included distortion and exchange effects in the solution near threshold of the equations¹ closely-coupling all the $n = 2$ states. The close-coupling results lie in general between Born and VPS treatments except at the lowest E . The agreement exhibited in fig. 2 between the VPS and close-coupling approximations for the $2^3S - 2^3P$ is remarkable. The singlet excitation cross sections are, in general, greater than those for the triplet excitations.

In figs. 3 and 4 are displayed the comparison of the Born cross sections with the VPS approximation (with effective-charge and exchange) for the singlet-singlet and triplet-triplet transitions to the $n = 3$ and 4 states. Convergence to the Born-limit is attained at high energies. The dip in the Born 3^3P and 4^3P cross sections at 10eV is a direct result of a zero occurring in the corresponding form-factors (7), and this dip is further reflected in the VPS curves

which are increasing with E at 10eV.

In conclusion, total excitation cross sections for transitions arising from electron-metastable helium transitions have been derived from two different approximations. In the Born approximation, the incident relative motion is represented by a plane wave unaffected by the target, while in the VPS method, the relative motion is taken as a product of two Coulomb waves arising from the incident electron-atomic electron repulsion and the incident electron-atomic core attraction. The differences exhibited in the various sets of cross-section curves is a measure of the importance of obtaining accurate wavefunctions for the relative motion. At present, the situation is difficult to assess without resort to more refined theoretical treatments as, for example, the close-coupling or multichannel eikonal approach⁹. However, in the absence of any experimental data and since the above two approximations correspond to the two extremes of relative motion, each set of curves in the figures simply display the present theoretical uncertainty in finding reliable cross sections for excitation out of metastable helium. Application of the VPS approximation to the $1s - 2s$ and $1s - 2p$ excitations and the ionization of atomic hydrogen by electron-impact does yield, however, cross sections^{3, 10} in good agreement with experiment. The agreement exhibited between the VPS and close-coupling methods for the $2^3S - 2^3P$ excitation is also encouraging.

However, all the figures clearly indicate the need that theoretical treatments more refined than above must closely-couple all the excitation channels together. The 3^1P cross section is smaller than both the 3^1D and 3^1S cross sections at low energies such that it would be affected by the presence of the $3^1D - 3^1P$ and $3^1S - 3^1P$ dipole couplings which would therefore tend to enhance the 3^1P excitation

at low energies. Thus for impact-energies $E < 100\text{eV}$, it is highly desirable to closely-couple all the 2^1S , 2^1P , 3^1S , 3^1P and 3^1D channels. Such an investigation would involve the solution of up to ten coupled differential equations and is quite difficult.

*This research was sponsored by the Air Force Aerospace Research Laboratories, Air Force Systems Command, United States Air Force, Contract F 33615-74-C-4003.

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* The authors wish to thank Dr. Y-K. Kim for sending us detailed tables of the form factors which were only partially given in reference 5.

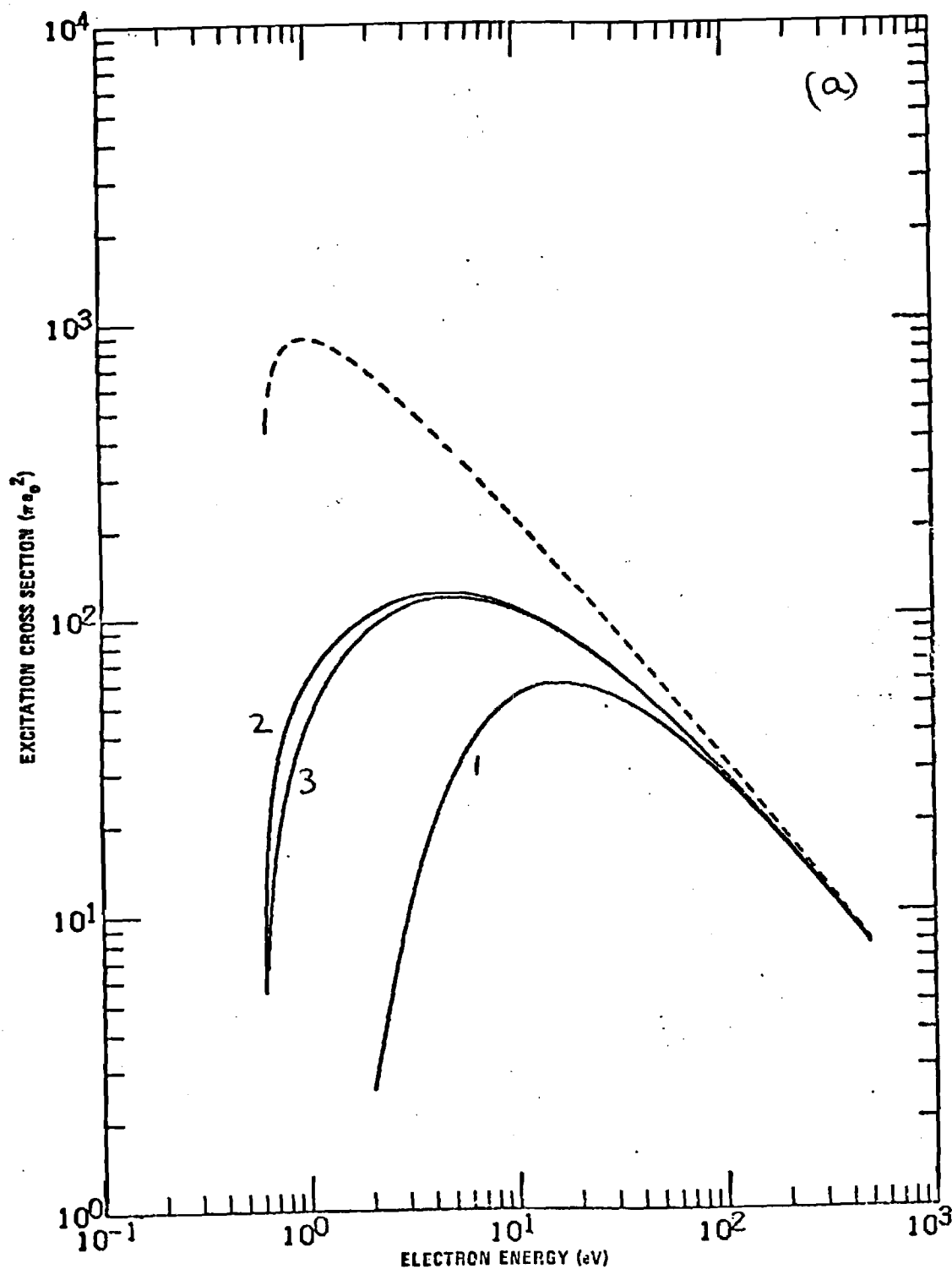


Figure 1 (a) The 2^1P and (b) the 3^1S cross sections for excitation arising from $e - \text{He}(2^1S)$ collisions as a function of electron impact-energy.

----: Born Approximation; eq. (6) in text

—: VPS Approximation; 1, 2 - eqs. (8) - (10) in text, with and without effective charge; 3 - eq. (18) with effective charge and exchange.

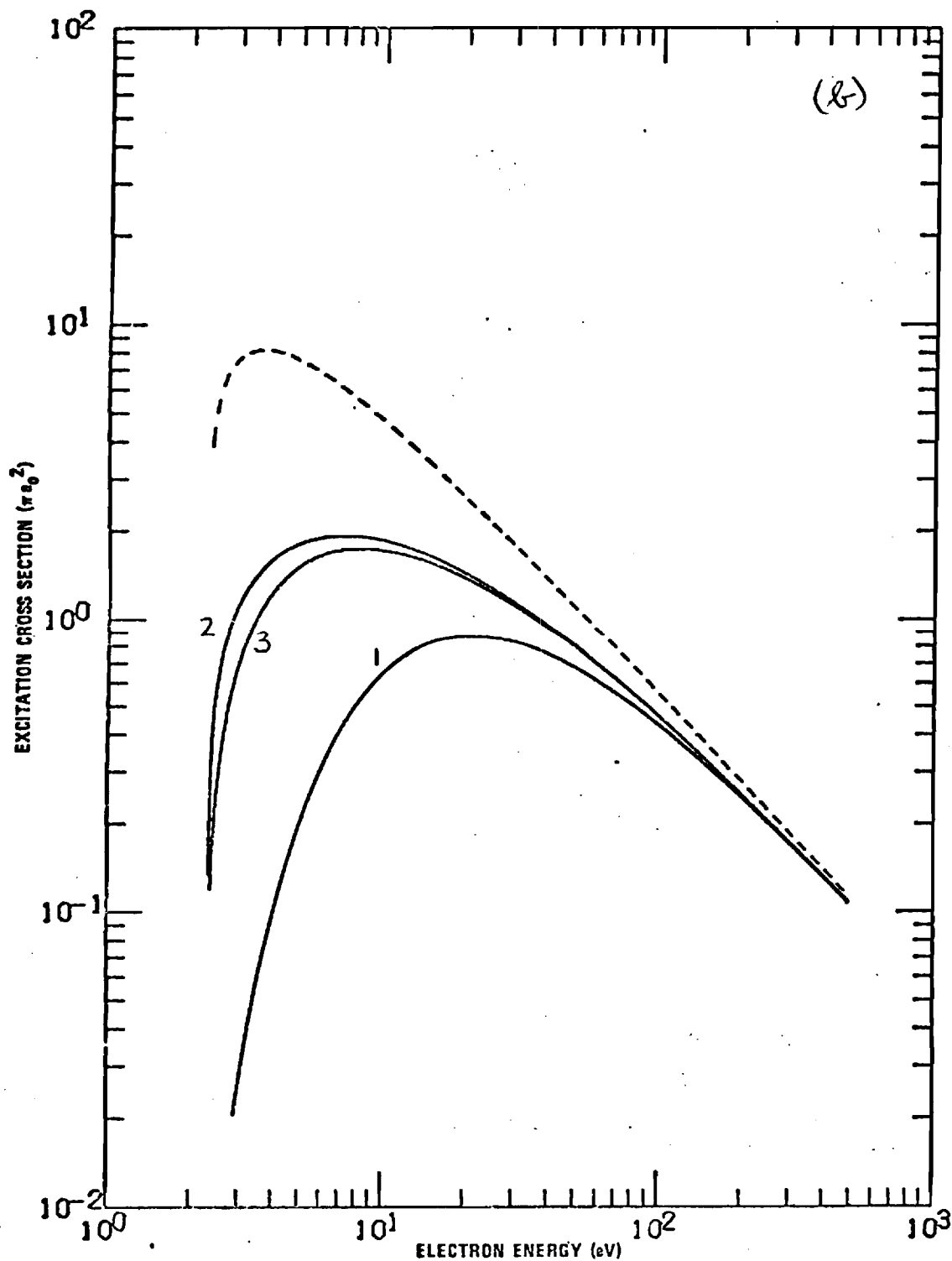


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---: Born Approximation; eq. (6) in text

—: VPS Approximation; 1, 2 - eqs. (8) - (10) in text, with and without effective charge; 3 - eq. (18) with effective charge and exchange.

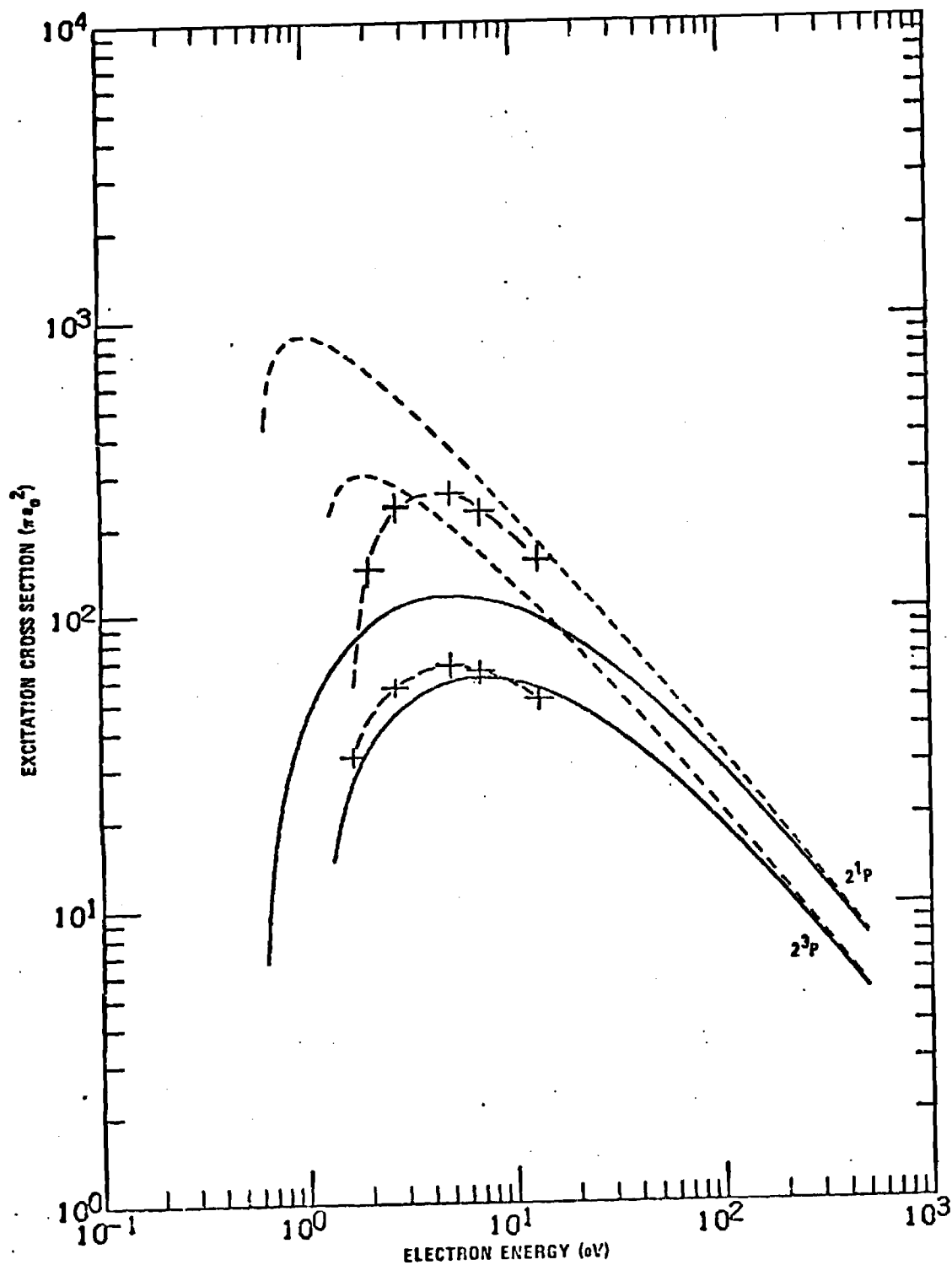


Figure 2 The $2^{1,3}P$ cross sections for excitation arising from $e - \text{He}(2^{1,3}S)$ collisions.

---: Born Approximation

—: VPS Approximation (3) with effective charge and exchange

--*: Close-coupling results of Burke et al.⁸

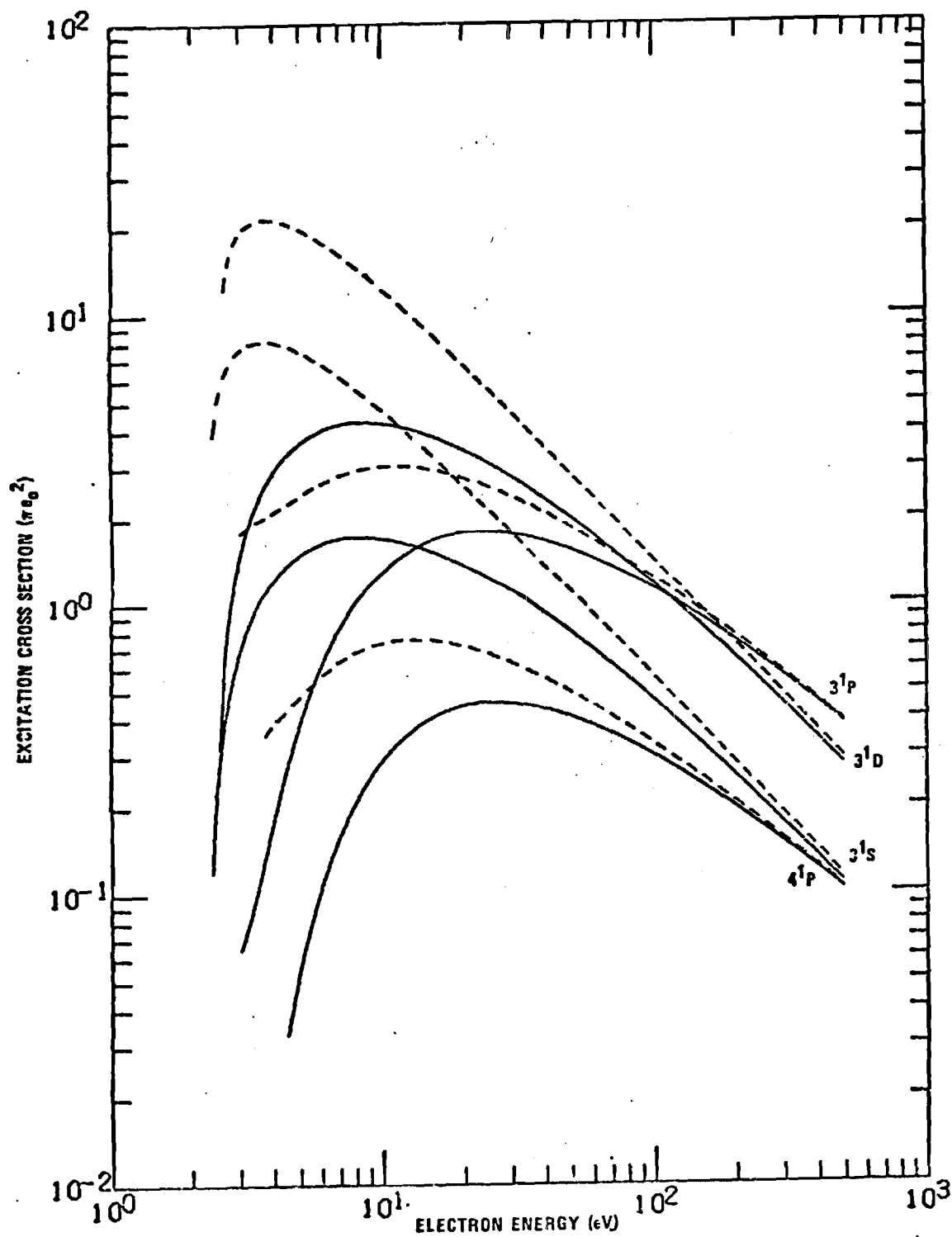


Figure 3 The 3^1S , 3^1P , 3^1D , and 4^1P excitations arising from $e - \text{He}(2^1S)$ collisions.
 ----: Born Approximation
 —: VPS Approximation (3) with effective-charge and exchange.

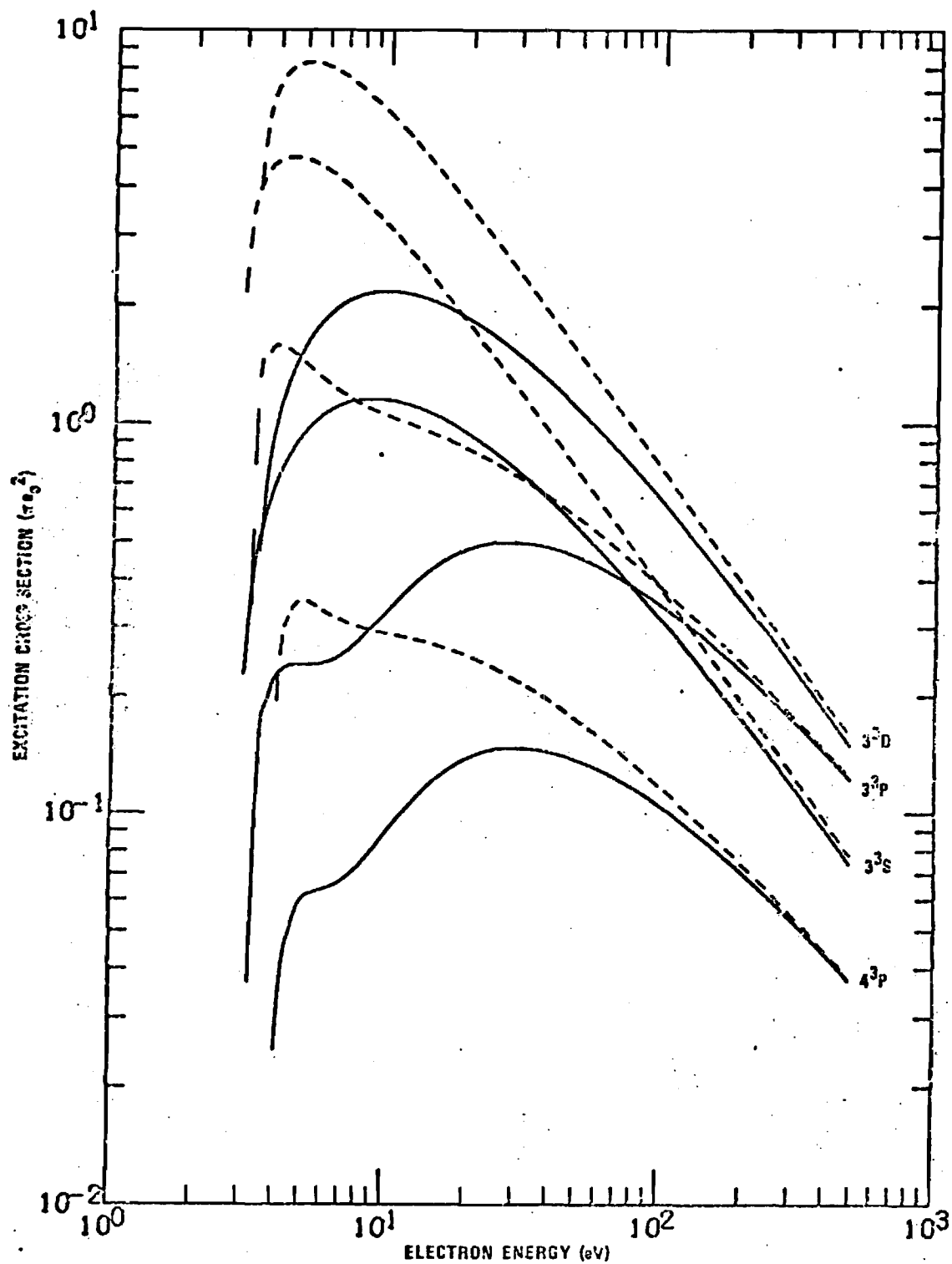


Figure 4 The 3³S, 3³P, 3³D, and 4³P excitations arising from e - He(2³S) collisions.

---: Born Approximation

—: VPS Approximation (3) with effective-charge and exchange.

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GEORGIA INSTITUTE OF TECHNOLOGY
ATLANTA, GEORGIA 30332

8 January, 1975

COL OF PHYSICS

Air Force Aerospace Research Laboratories

ATTN: ARL/DO

Contract F33615-74-C-4003

Item No. 0002, Sequence No.

Wright-Patterson AFB, OH 45433

SUBJECT: Quarterly R and D Status Report
Principal Investigator, M. R. Flannery
covering the period 8 Oct., 74 - 8 Jan., 75

Gentlemen:

Transmitted herewith are four (4) copies of the subject report.

Should you have any questions or comments regarding this report,
please contact the principal investigator.

Sincerely,

M. R. Flannery

M. R. Flannery
Professor

P.S. Six reprints of our published paper in Phys. Rev. A 10, 2264
(1974) are also enclosed.

MRF:jc
Enclosures

REPORT: Fifth Quarterly R & D Status Report
covering the period Oct. 8, 1974 - Jan. 8, 1975

PROJECT-TITLE: Calculation of Electron Impact Cross Sections
from Metastable States in Atomic and Molecular Gases

PRINCIPAL INVESTIGATOR: M. R. Flannery
School of Physics
Georgia Institute of Technology
Atlanta, Georgia 30332

CONTRACT NO: F33615-74-C-4003

SPONSOR CONTACT PERSON: Lt. John F. Prince / Dr. Alan Garscadden
U. S. Air Force
Air Force Systems Command
Bldg. 450, Area B
Hg. 4950th Test Wing, 4950 (PM MA)
Wright-Patterson, AFB, Ohio 45433

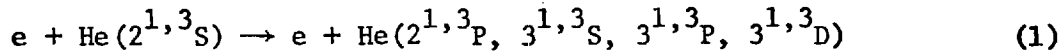
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1. Progress achieved during the period 8 Oct., 1974 - 8 Jan., 1975

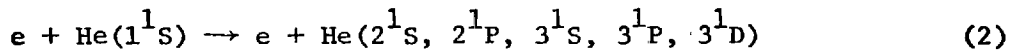
Summary. The following four projects were undertaken during the above period and are now completed:

- (1) Total excitation cross sections for the processes



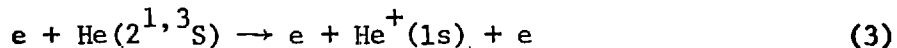
for electron-impact energies $E(\text{ev})$ in the range $5 \leq E \leq 200$ eV.

- (2) Total and differential excitation cross sections, and atomic orientation and alignment vectors for the processes



for electron-impact energies $E(\text{ev})$ in the range $40 \leq E \leq 500$ eV.

- (3) The semiquantal or binary encounter cross sections for the ionization processes



and

- (4) The Born approximation to the processes (3).

Further details of (1) - (4) are provided in section 5.

2. Publications in refereed scientific journals

The two manuscripts appearing as Appendices A and B of the previous status report no. 4, July 8, 1974 - Oct. 8, 1974 have been accepted for publication, and are now in press.

- (a) "A Pseudostate Multichannel Eikonal Study of $e - H(1s)$ Inelastic Collisions" by M. R. Flannery and K. J. McCann is to be published in J. Phys. B: Atomic and Molecular Physics (1975).
- (b) "Excitation in Electron-Metastable Helium Collisions" by M. R. Flannery, W. F. Morrison and B. L. Richmond is to be published in Journal of Applied Physics, March, (1975).

The above two papers bring the total number of papers published (or in press) and sponsored by this contract to six (6). In addition the progress summarized in section I will be eventually written up as three papers.

3. Presentations of papers at scientific meetings

- (a) "The Multichannel Eikonal Treatment of Electron-Atom Collisions". Long paper delivered at the 27th Annual Gaseous Electronics Conference (GEC), Houston, Texas, October 22-25, 1974.
- (b) "The Multichannel Eikonal Treatment of Electron-Helium Collisions". Paper delivered at the 6th Annual Meeting of the Division of Electron and Atomic Physics (DEAP), Chicago, December 2-4, 1974.
- (c) "The Multichannel Eikonal Treatment of Electron-Hydrogen Collisions". Delivered at the 1974 Fall General Meeting of the American Physical Society (APS), Atlanta, December 5-7, 1974.

The executive secretary Dr. W. W. Havens, Jr. of the American Physical Society has invited Dr. Flannery to address the APS at its 1975 Annual Meeting in Anaheim, California, 29 January - 1 February, 1975. The title of Dr. Flannery's invited paper is entitled "The Role of Highly Excited Rydberg States in Astrophysics" and is scheduled for thirty minutes in a session entitled "Atomic and Molecular Physics Problems in Astrophysics". Although this work is not being sponsored by the Air Force, there are however many similarities between the roles played by excited states in laboratory and astrophysical plasmas. The abstract appears in page 4.

American Physical Society

29 January - 1 February 1975

Date

The Role of Highly Excited Rydberg States in Astrophysics
M. R. FLANNERY, School of Physics, Georgia Institute of Technology, Atlanta (30 min.)

The radiofrequency emission spectrum of gaseous nebulae such as Orion A and NGC 2024 is attributed to radiative transitions between atomic (and molecular) states with a very high principal quantum number (e.g. H110 α , He109 α , He137 β). These highly excited levels are mainly populated by radiative, dielectronic and three-body recombinations between electrons and ions produced by photoionization of the neutrals by stellar ultraviolet radiation. The excited levels are subsequently formed and destroyed by spontaneous downward transitions resulting in radiofrequency recombination lines, and by collisional ionization and excitation. Observations¹ of the H157 α line and neighboring frequencies yield spectra arising from two regions with different physical characteristics -- (1) broad spectra of H and He formed in HII regions ($T_e \sim 10^4$ K, $n_e \sim 10^4$) and (2) anomalous spectra (narrower than (1) by a factor 4 - 7) due to C157 α , originating in HI regions ($T_e \sim 5 - 100$ K, $n_e \sim 1$, $n_H \sim 10^3$) under non-LTE conditions and stimulated by a background continuum provided e.g. by HII regions. The detailed analysis of such spectra requires the knowledge of cross sections for collisional excitation and ionization of highly excited species by electrons and neutrals. Moreover, for the low temperature HI regions, in particular, molecular species (e.g. CO) exist, with the possibility that rotational excitation can occur² via a resonance transfer of electronic energy by a collision with the highly excited atoms. The rates for these collisions can become much larger than those neutral-neutral collisions which involve no rotational changes. Penning ionization effects may also be important. Properties of excited states will be examined and theoretical models for various collisional processes involving excited states will be presented and illustrated.

¹J. A. Ball, D. Cesarsky, A. K. Dupree, L. Goldberg and A. E. Lilley, Ap. J. (Letters) 162, L25 (1970)

²M. R. Flannery, Ann. Phys. (N. Y.) 79, 480 (1973)

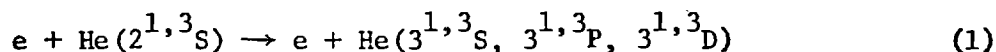
4. Awards

Dr. Flannery was awarded the Monie A. Ferst Award by Sigma Xi for outstanding research in 1973. Dr. Flannery's list of publications to date appear as Appendix A.

5. Results

Project 1

During this contract period 8 Oct., 1974 - 8 Jan., 1975, total excitation cross sections for the processes



were calculated for electron-impact-energies $E(\text{eV})$ in the range $5 \leq E \leq 200$.

A ten-channel Eikonal approximation was applied to this investigation in which the 1^1S , 2^1S , 2^1P , 3^1S , 3^1P and 3^1D channels were closely coupled for the singlet excitations and all except 1^1S for the triplet excitations. The total cross sections are displayed in figures 1 - 3. This study represents a major development and fundamental breakthrough in the examination of electron-excited atom collisions and was possible only after much systematic research and recognition of several important effects important for excited atoms.

Points to be noted from figures 1 - 3

(a) The $2^{1,3}\text{S} - 2^{1,3}\text{P}$ transitions dominate all the inelastic excitations by at least an order of magnitude. The agreement between our present $2^{1,3}\text{P}$ cross sections and those of Burke, Cooper and Ormonde (Phys. Rev. 183 (1969) 245) is very good. In addition the Born approximation (with extremely accurate 50-parameter wavefunctions) is in very close agreement for impact-energies $E > 30 \text{ eV}$ in figure 1. This observation indicates that Born's approximation is in fact valid down to much lower impact-energies E for excitation from excited states than from ground-states of atoms. This observation is in accord with the facts that the validity criterion of Born's approximation is $E \gg \Delta E$ where ΔE is the excitation energy which is very small for initial excited states compared with initial ground states.

(b) In figures 2 and 3, the $2^{1,3}S - 3^{1,3}D$ transition yields the dominant contribution to $n = 3$ excitation except at high energies (> 100 and 1000 eV for singlet and triplet transitions respectively). The order of importance is $2^{1,3}S - 3^{1,3}D$, $2^{1,3}S - 3^{1,3}S$, $2^{1,3}S - 3^{1,3}P$ in descending order at low energies.

(c) While the Born approximation fails for $E < 20\text{eV}$, it is in very good accord with the more elaborate study at higher energies.

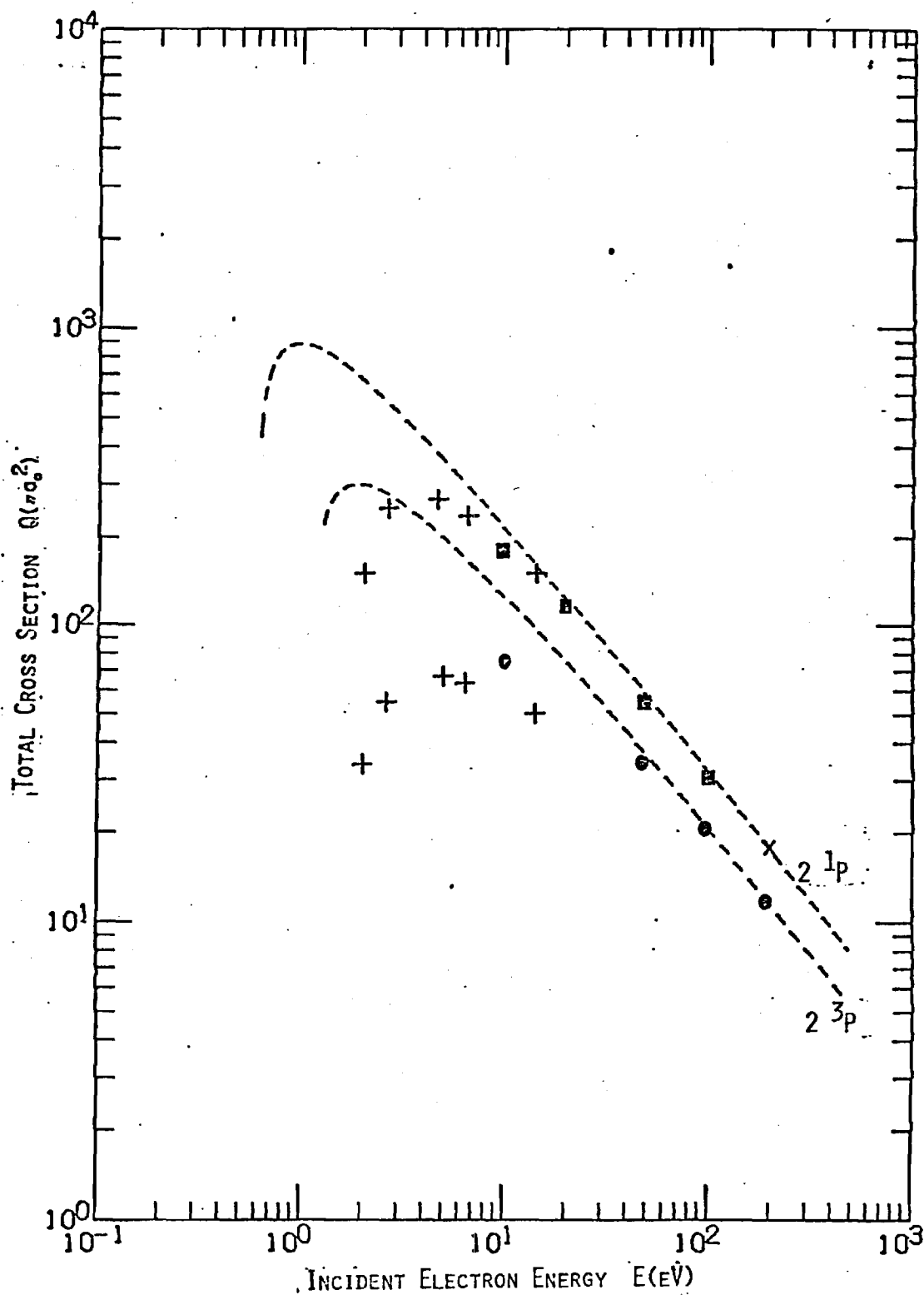
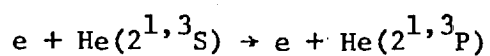


Figure 1: Total excitation cross sections for the process



at electron energy E (eV). , : present ten-channel eikonal treatment. + Burke et al (1969). ---- Born approximation.

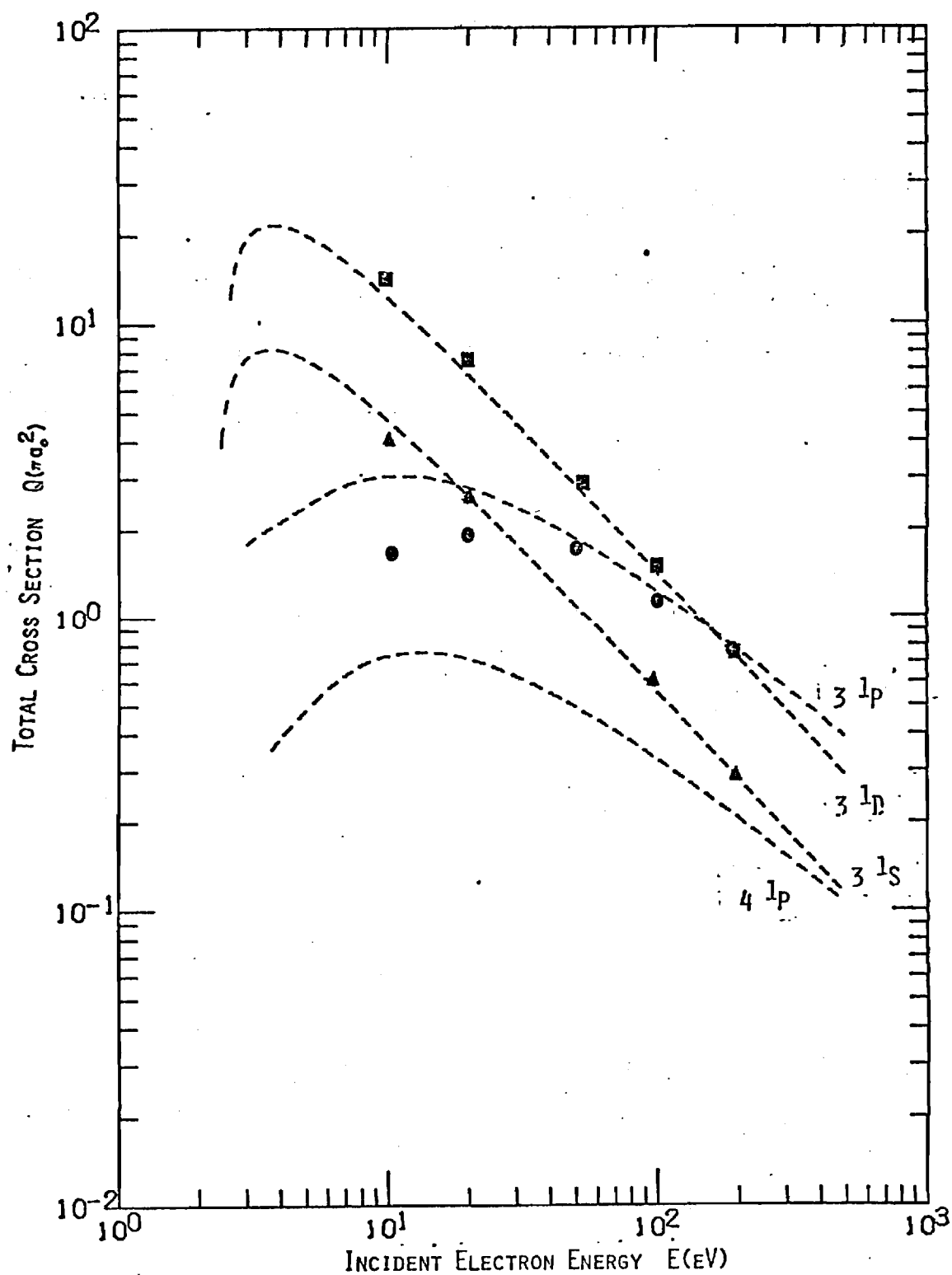
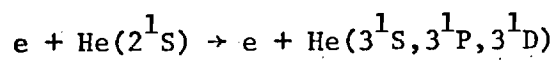


Figure 2: Total excitation cross sections for the processes



at electron energy $E(\text{eV})$. , , : present ten-channel eikonal treatment. ---- Born approximation.

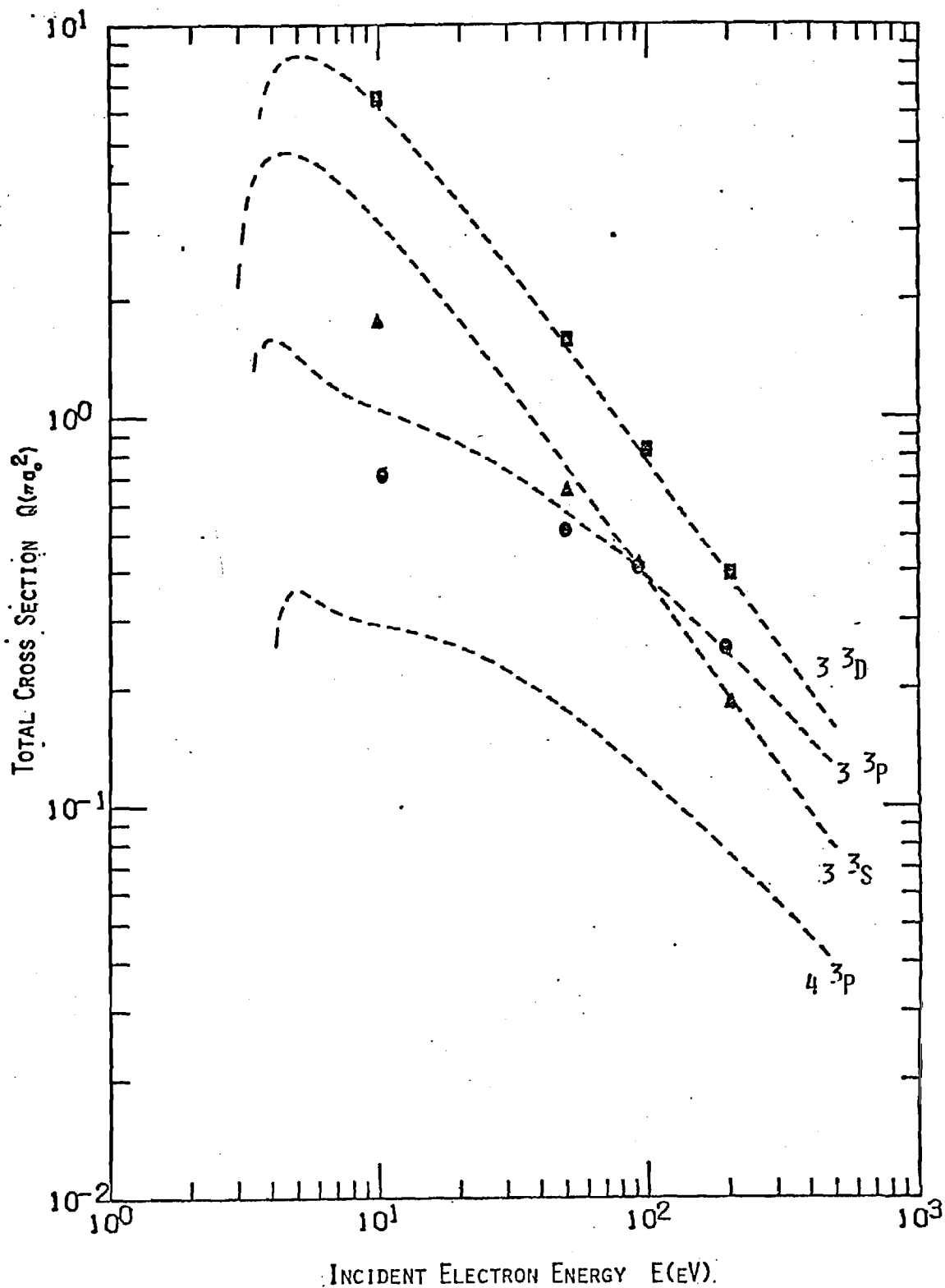
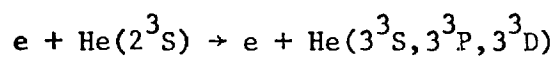


Figure 3: Total excitation cross sections for the processes



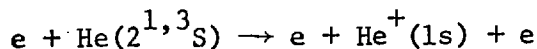
at electron energy E (eV). , , : present ten-channel eikonal treatment. ---- Born approximation.

Projects 2 and 3

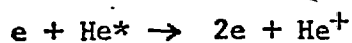
In view of the close agreement between the Born and the more elaborate multichannel eikonal cross sections for $e - \text{He}(2^{1,3}\text{S})$ excitation collisions, cross sections for ionization out of the metastable He states were calculated. Ionization is an extremely difficult problem (compared with excitation) and information on approximations is scant. The application of Born's approximation is difficult and lengthy and involves the calculation of a four-dimensional integral for helium for each impact-energy. Moreover, a continuum orbital for the ejected electron has to be calculated at each angular momentum l at each momentum change K and at each energy of the ejected electron.

Because the atom is initially in an excited state such that the valence electron is quite distant from the He^+ core ($\langle r_{12} \rangle \approx 5a_0$ for He), a binary-encounter method was also applied.

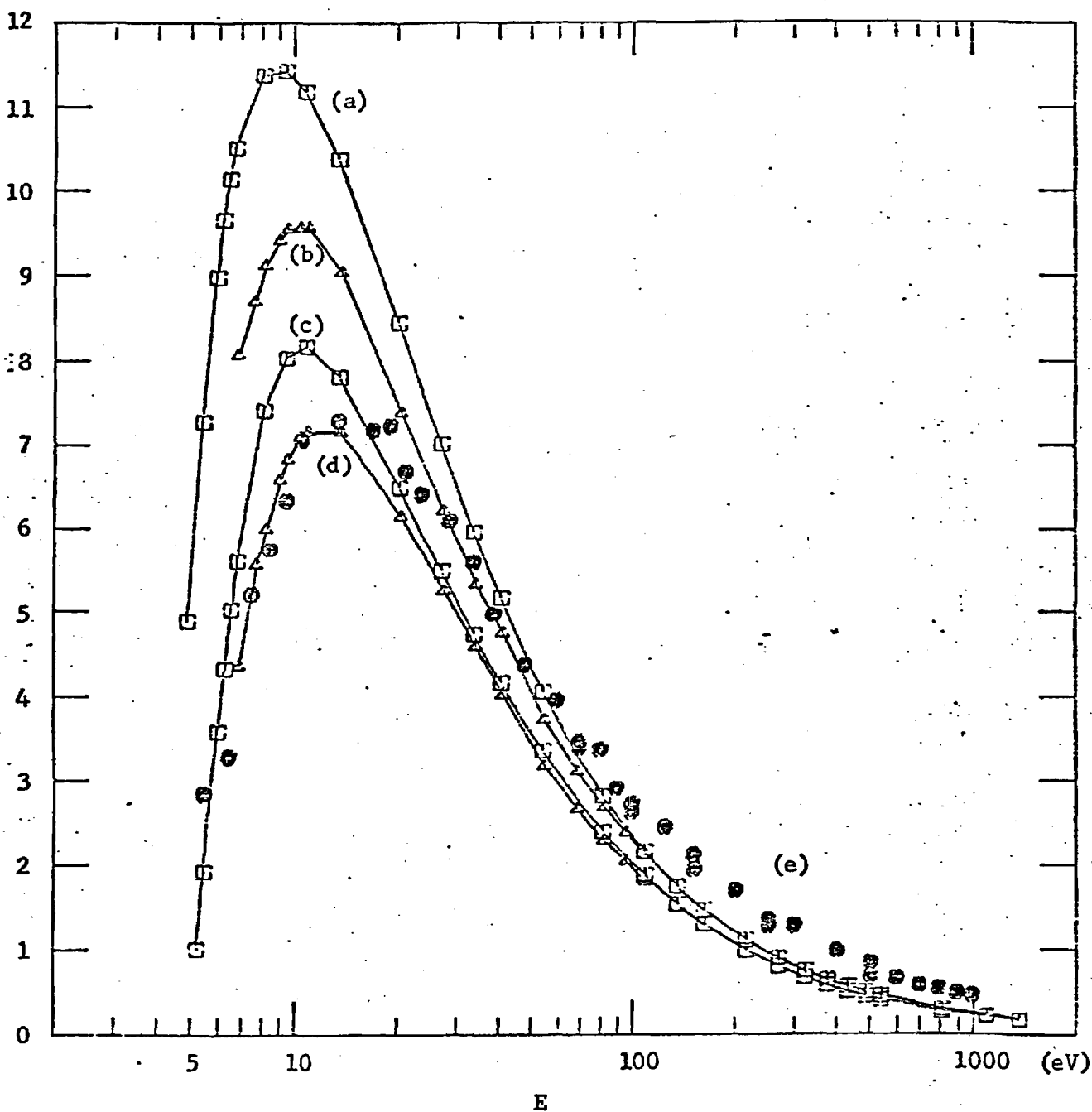
In figure 4, preliminary results are displayed for the cross sections of the ionizations



Experimental results of Harrison, Smith and Dixon (supplied to me in advance of publication) are also included. In view of the uncertainty in experiment, the agreement particularly at the lower energies, is very good.



Total Cross-section for electron-impact ionization vs. incident electron energy



- Figure 4: (a) $21s$: calculated by the binary encounter method using the Coh.&McE. wfn.
 (b) $21s$: -- Born approximation using solns. of H-S potl. for He gd. 'st
 (c) $23s$: -- binary encounter method using the Coh.&McE. wfn.
 (d) $23s$: -- Born approximation using solns. of H-S potl. for He exc. s
 (e) Experimental data of Dixon et al. for a predominantly $23s$ target.

Project 4

During the past year of our research, it has already been established that the multichannel eikonal method developed by Flannery and McCann has yielded

(a) total and differential cross sections for collisional excitation involving electrons and ground-state atoms which agreed very closely with other refined theoretical results and experiment. In most instances, the present method provided cross sections which either were in better accord with experiment than other theoretical values or else were the only refined theoretical values in existence. Electron-hydrogen and electron-helium collisions were thoroughly explored and the method well-tested before proceeding to electron-excited atom collisions. The chief advantage of the method, is its general applicability to electron-excited atom collisions. It is without the disadvantages associated with application of the standard methods designed with ground-state atoms in mind.

However as a further and very definitive test of the model, orientation and alignment vectors were calculated for e - He collisions. These vectors are more basic to the collision than are the total and differential cross sections, and have for the first time been measured in a striking experiment recently reported by Kleinpoppen et al. in J. Phys. B. 12, 1519-1542 (1974). This work is extremely important in that it provides tests of the collision model, much more sensitive than even the total and differential cross sections. A full report on our work is contained in Appendix B.

6. Personnel involved in the research

- (a) M. R. Flannery, Professor of Physics - Principal Investigator
- (b) Dr. K. J. McCann, Postdoctoral Fellow
- (c) Dr. D. T. That, Postdoctoral Fellow
- (d) Mr. W. R. Morrison, Graduate Student

Appendix A: Biographical Sketch

BIOGRAPHICAL SKETCH

Name: Martin R. Flannery

Rank: Professor of Physics

Birth Date: January 8, 1941

Education:

B.Sc., (First Class Honors) The Queen's University of Belfast, N. Ireland, 1961

Ph.D., The Queen's University of Belfast, N. Ireland, 1964

Employment History (since award of highest degree):

Assistant Lecturer, Queen's University, 1964-66

Research Associate, Joint Institute for Laboratory Astrophysics, 1966-67

Assistant Professor of Physics, Georgia Institute of Technology, 1967-68

Associate, Harvard College Observatory, 1968-70

Physicist, Smithsonian Astrophysical Observatory, 1968-71

Lecturer, Harvard University, 1970-71

Associate Professor of Physics, Georgia Institute of Technology 1971-1974

Professor of Physics, Georgia Institute of Technology, 1974-present

Current Fields of Interest:

Theoretical Physics. Theoretical studies of atomic and molecular processes with applications to aeronomy, astrophysics, and the laboratory; the interpretation of the atmospheres on the Earth, Mars, and Venus and of the interstellar medium. Basic research in collisional excitation and ionization of atoms and molecules by electron and atom impact and in ion molecule reactions.

Professional Activities; Memberships in Professional Societies:

Member, Institute of Physics, London

Member, American Physical Society

Member, Sigma Xi

Awards:

Certificate of Academic Achievement, in recognition of distinguished accomplishment in higher education and research. Awarded by the Smithsonian Institution, Washington, D. C., July, 1972.

Monie A. Ferst Award given by Sigma Xi (Georgia Tech Chapter) for outstanding research in 1973.

Selected Publications:

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18. "The 2s and 2p Excitations of Hydrogen by Proton and Helium-Ion Impact," J. Phys. B (Atom. Molec. Phys.), 2, 1044-54 (1969).
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20. "Single and Double Excitations in Hydrogen-Hydrogen Excitation Collisions," with H. Levy, II, J. Phys. B (Atom. Molec. Phys.), 3, 121-3 (1970).
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22. "Inclusion of Higher State Couplings in a Multistate Impact-Parameter Treatment of Heavy-Particle Collisions," J. Phys. B (Atom. Molec. Phys.), 3, 789-803 (1970).
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Appendix B: Project 4

1. Introduction

The study of angular correlations between the emitted photon and scattered electron in inelastic electron-atom collisions has permitted the measurement of complex transition amplitudes and atomic orientation and alignment vectors (Macek and Jaecks 1971, Fano and Macek 1973) from parameters written as λ and χ by Eminyan et al. (1974). These collision parameters λ and χ are more basic than total cross section σ , differential cross section $d\sigma/d\Omega$, or even percentage polarization P of the emitted radiation. They have generally been "hidden" in most refined theoretical calculations of the collision and "lost" in experiments designed to measure σ and P alone. By the use of delayed coincidence techniques, Eminyan et al. (1974) have conducted striking experiments from which this basic information on λ and χ can be extracted without the need for normalization.

This work together with the measured $d\sigma/d\Omega$ of e.g. Trajmar (1973) and σ of e.g. Donaldson et al. (1972) all provide excellent tests of the various theoretical models recently developed for electron-atom collisions at intermediate impact-energies E (see the review of McDowell 1975). For example, in spite of its apparent success for σ and $d\sigma/d\Omega$, the Glauber approximation exhibits serious deficiencies in its predictions of λ and χ . These shortcomings are directly attributable to gross simplifications such as the assumption of a heavy-particle and high-energy limit in the collision dynamics.

In this paper, the multichannel eikonal approach of Flannery and McCann (1975) which pays particular attention to the collision dynamics is further tested by examining the variation of λ , χ , and $d\sigma/d\Omega$ with θ and E and of σ and P with E for the inelastic collisions,

$$e + \text{He}(1^1\text{S}) \rightarrow e + \text{He}(n^1\text{L}), \quad n = 2, 3; \quad L = \text{S, P, D.} \quad (1)$$

All ten channels of (1) will be closely-coupled and the accurate frozen-core Hartree-Fock wavefunctions of Cohen and McEachran (1974) will be used throughout.

2. Theory

2.1 Basic Formulae

The key quantity sought in theoretical descriptions of atomic collisions is $f_{if}(\theta)$, the complex scattering amplitude as a function of scattering angle θ (in the CM-frame) and of impact-energy E for various $i \rightarrow f$ transitions occurring in the collision species with initial and final relative momenta \underline{k}_i and \underline{k}_f respectively. For a non-degenerate initial state i , experiment yields (a) the differential cross section

$$\frac{d\sigma}{d\Omega} = \frac{k_f}{k_i} \sum_{M=-L}^L |f_{if}^{(M)}(\theta)|^2 \quad (2)$$

summed over all degenerate magnetic substates M of the final state f of the target with angular momentum L , (b) the associated total cross section σ and (c) the polarization fraction P which determines the relative contribution arising from each M to the total σ . In a recent experiment on the $1^1S - 2^1P$ collisional excitation of He by e, Eminyan et al. (1974) measured, as functions of θ and E , the additional parameters

$$\lambda = |f_{if}^{(0)}|^2 / [|f_{if}^{(0)}|^2 + 2|f_{if}^{(1)}|^2] \quad (3)$$

and

$$|\chi| = |\alpha_1 - \alpha_0| \quad (4)$$

where α_M is the phase of the scattering amplitude

$$f_{if}^{(M)} = |f_{if}^{(M)}| e^{i\alpha_M} \quad (5)$$

and where the axis of quantization is taken along the incident Z-direction defined by \hat{k}_i .

The quantity λ is the relative contribution arising from the $M = 0$ substate to $(d\sigma/d\Omega)$ in (2), while χ is a measure of the coherence between the excitations of the $M = 0$ and 1 substates. A related quantity is the circular polarization fraction of radiation emitted perpendicular to the (assumed) XZ-plane of the scattering,

$$\Pi = -2 [\lambda(1 - \lambda)]^{1/2} \sin \chi \equiv \overline{\Delta L_Y} \equiv L(L + 1) O_{1-}^{\text{col}} \quad (6)$$

where $\overline{\Delta L_Y}$ is the expectation value of the angular momentum transferred in the Y-direction during the collision and where O_{1-}^{col} is the orientation vector (cf. Fano and Macek 1973, Eminyan et al. 1974).

The overall accuracy of a particular theoretical collision-model can therefore be assessed by the closeness between theoretical calculations and experimental measurements of the three independent quantities $d\sigma/d\Omega$, λ and χ as functions of θ and E . For example, the Born approximation predicts that $\lambda_B = \cos^2(\hat{K} \cdot \hat{k}_i)$ for S - P transitions, since $f_{if}^{(M)} \propto |Y_{1M}(\hat{K})|^2$ is a function only of the momentum-change $\underline{K} \equiv (K, \theta, \phi) = \underline{k}_i - \underline{k}_f$, and that $\chi_B = 0$, since $f_{if}^{(M)}$ is always real. The Π -polarization is therefore zero. The prescription of Glauber(1959) involved setting $\underline{K} \cdot \underline{k}_i = 0$ so as to ease subsequent calculation with the result that $f_{if}^{(0)}$ and hence λ_G vanish. Also $\alpha_{\pm 1} = \pm i\phi$ and so $\chi_G = 0$. By adopting a change of Z-axis, however, along $\frac{1}{2}(\underline{k}_i + \underline{k}_f)$ such that K_Z in this direction is identically zero and by following the analysis of Gerjuoy et al. (1972), then it can be shown that, for S - P transitions, $\lambda_G = \cos^2(\hat{K} \cdot \hat{k}_i)$ in harmony with the first Born approximation. Therefore in spite of its relatively better performance in evaluating both σ and $d\sigma/d\Omega$, the Glauber approximation is at least worse or at best equal to the Born predictions of λ and χ .

In the present investigation, the multichannel eikonal description (Flannery and McCann 1975) is applied to the examination of σ , $\frac{d\sigma}{d\Omega}$, P , λ and χ for the $n = 2$

and 3 excitations of helium by electron impact. In this treatment, the complex amplitude for scattering with final relative momentum \underline{k}_f in direction (θ, ϕ) with respect to polar axis along the direction of incident relative momentum \underline{k}_i is, in the CM-frame,

$$f_{if}(\theta, \phi) = -i^{\Delta+1} \int_0^\infty J_\Delta(K'\rho) [I_1(\rho, \theta) - i I_2(\rho, \theta)] \rho d\rho \quad (7)$$

where J_Δ are Bessel functions of integral order $(M_i - M_f)$ and where K' is the XY-component $k_f \sin \theta$ of the momentum-change $\underline{K} = \underline{k}_i - \underline{k}_f$. The collision functions

$$I_1(\rho, \theta; \alpha) = \int_{-\infty}^\infty K_f(\rho, Z) \left[\frac{\partial C_f(\rho, Z)}{\partial Z} \right] \exp(i\alpha Z) dZ \quad (8)$$

and

$$I_2(\rho, \theta; \alpha) = \int_{-\infty}^\infty \left[K_f(K_f - k_f) + \frac{\mu}{\hbar^2} V_{ff} \right] C_f(\rho, Z) \exp(i\alpha Z) dZ \quad (9)$$

contain a dependence on the scattering angle θ via

$$\alpha = k_f(1 - \cos \theta) = 2k_f \sin^2 \frac{\theta}{2} \quad (10)$$

the difference between the Z-component of the momentum change \underline{K} and the minimum change $k_i - k_f$ in the collision. The coupling amplitudes C_f are solutions of the following set of N-coupled linear equations

$$\frac{i\hbar^2}{\mu} K_f(\rho, Z) \frac{\partial C_f(\rho, Z)}{\partial Z} + \left[\frac{\hbar^2}{\mu} K_f(K_f - k_f) + V_{ff}(\rho, Z) \right] C_f(\rho, Z) = \sum_{n=1}^N C_n(\rho, Z) V_{fn}(\rho, Z) \exp i(k_n - k_f) Z, \quad f = 1, 2, \dots, N \quad (11)$$

solved subject to the asymptotic boundary condition $C_f(\rho, -\infty) = \delta_{if}$. The local wavenumber of relative motion at separation $\underline{R} \equiv (R, \theta, \phi) \equiv (\rho, \phi, Z)$ is $K_n(\underline{R}) = [k_n^2 - \frac{2\mu}{\hbar^2} V_{nn}(\underline{R})]^{\frac{1}{2}}$ where the interaction matrix elements $V_{nm}(\underline{R}) = \langle \psi_n(\underline{r}_1, \underline{r}_2) | V(\underline{r}_1, \underline{r}_2, \underline{R}) | \psi_m(\underline{r}_1, \underline{r}_2) \rangle$ connect the various electronic states $\psi_n(\underline{r}_1, \underline{r}_2)$ of atomic helium and where V is the instantaneous e - He electrostatic interaction.

It can be shown directly that, at high energies, the basic equations satisfy the optical theorem,

$$\sum_f \sigma_{if} = \frac{4\pi}{k_i} \text{Im } f_{ii}(0) \equiv 4\pi \int_0^\infty (\text{Re } C_i - 1) \rho \, d\rho = 2\pi \sum_f \int_0^\infty |C_f - \delta_{if}|^2 \rho \, d\rho \quad (12)$$

Verification, however, for all impact-energies is not as straightforward and would require direct numerical evaluation of all the cross sections.

2.2 Wavefunctions and Interactions

All ten channels of (1) will be closely coupled. We adopt the frozen-core Hartree-Fock $n = 1 - 3$ helium wave-functions of Cohen and McEachran (1974) in the form

$$\psi_{1s,n\ell m}(\underline{r}_1, \underline{r}_2) = N_{n\ell} [\phi_o(\underline{r}_1) \phi_{n\ell m}(\underline{r}_2) + \phi_o(\underline{r}_2) \phi_{n\ell m}(\underline{r}_1)] \quad (13)$$

in which the frozen, inner $1s$ -orbital is (in a.u.)

$$\phi_o(\underline{r}) = 2^{5/2} e^{-2r} Y_{00}(\hat{\underline{r}}) \quad (14)$$

and the orbital for the second electron in state $(n\ell m)$ is rewritten (in a.u.) as,

$$\phi_{n\ell m}(\underline{r}) = \sum_{N=\ell+1}^{J-\ell} B_N^{n\ell} e^{-\beta r} r^{N-1} Y_{\ell m}(\hat{\underline{r}}), \quad \beta = \frac{2}{n} \quad (15)$$

where J is the maximum number of linear coefficients $B_N^{n\ell}$ given in terms of Cohen and McEachran's original parameters $a_j^{n\ell}$ by

$$B_N^{n\ell} = \sum_{j=N+\ell}^J \frac{(-1)^{N-\ell} 2^\ell (j!)^2 (2\beta)^{N-\ell-1}}{(N-\ell-1)!(j-N-\ell)!(N+\ell)!} a_j^{n\ell}, \quad N = 1, 2, \dots, J \quad (16)$$

The above transformation (16) facilitates subsequent evaluation of the $e - \text{He}$ interaction matrix elements

$$V_{ij}(R) = \langle \phi_i(\underline{r}_1, \underline{r}_2) \left| -\frac{2}{R} + \frac{1}{|\underline{R} - \underline{r}_1|} + \frac{1}{|\underline{R} - \underline{r}_2|} \right| \phi_j(\underline{r}_1, \underline{r}_2) \rangle \quad (17)$$

as analytical functions of R such that the exponential and linear parameters α_i

and a_s in the resulting expression,

$$V_{n\ell m, n'\ell' m'}(R) = \sum_{L=|\ell-\ell'|}^{(\ell+\ell')} \left[-\frac{a_{-t}}{R^t} + \sum_{i=1}^2 e^{-\alpha_i R} \sum_{s=-t}^{16} a_s R^s \right] Y_{LM}(R) \quad (18)$$

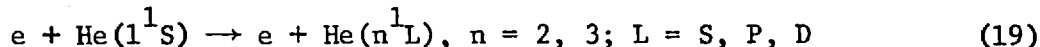
can be determined exactly and automatically.

2.3 Test of wavefunctions

Theoretical refinement to the collision model must be accompanied whenever possible by accurate atomic wavefunctions since the goodness thereby introduced by the former may be completely swamped by an inappropriate choice of wavefunctions (cf. McCann and Flannery 1974). The overall reliability of the present set of wavefunctions has already been gauged by examination of associated eigenenergies and cusp conditions (Cohen and McEachran 1967, McEachran and Cohen 1969). In this investigation, the present set of wavefunctions did reproduce the accurate Born results of Bell et al. (1969) for the $n = 2$ and 3 excitations of He. However, it is worth noting that similar reproductions were achieved for the $n = 4-6$ He-excitations, only when one adopted additional linear parameters $a_j^{n\ell}$, which were not contained in the above cited references (so as to economize in table presentation), but which were obtained from Cohen and McEachran (1974) privately. Therefore, in all the present calculations we have employed the twenty-parameter functions provided by Cohen and McEachran (1974). The non-orthogonality integrals $\langle \psi_i | \psi_f \rangle$ were found to be negligible for all channels.

3. Results and Discussion

A ten-channel eikonal description (7) - (11) was carried out for the inelastic collisions



and the parameters $d\sigma/d\Omega$, λ and χ determined from (2) - (5) as functions of scattering angle θ for various impact energies $E(\text{eV})$ in the range $40 \leq E \leq 500$. A four-channel (1^1S , 3^1S , $3^1\text{P}_{0,\pm 1}$) treatment was also performed.

3.1 Total Cross Sections and Polarization Fractions

Total excitation cross sections

$$\sigma(E) = 2\pi \frac{k_f}{k_i} \int_0^\pi |f_{if}(\theta)|^2 d(\cos \theta) \quad , \quad (20)$$

are displayed in figures (1 - 4) for each transition in (19), together with comparison experimental and theoretical data. These figures include results from the following recent theories:

- (a) The second-order potential treatments (S) of Berrington et al. (1973) for the $n = 2$ excitations and of Bransden and Issa (1974) for the $n = 3$ excitations,
- (b) The second-order diagonalization procedure of Baye and Heenen (1974),
- (c) The first-order many-body approach (M) of Thomas et al. (1974) for the $n = 2$ excitations,
- (d) A four-channel eikonal (E4) study (McCann and Flannery 1974) of the $n = 2$ excitations,
- (e) The Glauber treatment of Chan and Chen (1973, 1974 a, b) for the $n = 2$ and 3^1P excitations,
- (f) The Born results B of Bell et al. (1969).

The experimental data are taken from Rice et al. (1972), Vriens et al. (1968), Miller et al. (1968), Donaldson et al. (1972), de Jongh and van Eck (1971) and Moustafa Moussa et al. (1969). Since figures (1 - 4) provide a rather detailed comparison, only a few comments are needed. In general, the present ten-channel results E10 are in good accord with experiment. Couplings with the $n = 3$ channels are very important for the 2^1S excitation at all energies, although the 2^1P cross section is essentially left unaffected. The 2^1P distorted Born-wave results (not shown) of Madison and Sheldon (1973) are indistinguishable from the present E10 curve. Cross sections in excess of the Born values are obtained only for the 3^1D excitation in figure (3b), when the $3^1P - 3^1D$ dipole coupling becomes extremely important and causes the enhancement at the lower energies. Note that the Born limit remains unattained even at 500 eV for the n^1S excitations in figures 1 and 3a, although the n^1P and 3^1D cross sections show fairly rapid convergence from below and above respectively onto the corresponding Born limits.

The present ten-channel cross sections σ_M for excitation of magnetic sublevel M of (19) are presented in table 1 together with the four-channel and Born values at 500 eV. The percentage polarization fractions

$$P(n^1P) = \frac{\sigma_o - \sigma_1}{\sigma_o + \sigma_1} \quad (21)$$

and

$$P(3^1D) = \frac{3(\sigma_o + \sigma_1 - 2\sigma_2)}{5\sigma_o + 9\sigma_1 + 6\sigma_2} \quad (22)$$

for the radiation emitted from the n^1P and n^1D states respectively (Percival and Seaton 1958) are displayed in table 2. For high $E \geq 300$ eV, $P(2^1P) \approx P(3^1P)$.

3.2 Differential Cross Sections

These provide a more sensitive test of the present theory and representative cases are displayed in figures 5 and 6 for the 2^1S and 2^1P excitations as a function of scattering angle θ at two incident energies 40 eV and 80 eV. (Computer printouts of the remainder at all the energies in table 1 are available from the authors upon request).

Examination of the figures 5 and 6 shows that the present multichannel model is generally quite successful in describing inelastic scattering about the forward direction up to $\theta \approx 40^\circ$. In particular, as indicated by fig. 5a the many-body treatment of Thomas et al. (1974) fails quite markedly, by comparison, to reproduce the measurements of Trajmar (1973) in this angular range for the 2^1S excitation. This shortcoming is presumably attributed to the fact that their first-order approach has neglected the $2^1S - 2^1P$ dipole coupling which strongly enhances the 2^1S scattering about the forward direction. The 2^1P cross section is affected much less by the presence of this coupling, as shown by figure 6. With increasing E , the scattering becomes more concentrated in the forward direction and is therefore well described by the present model.

Although the present version of the multichannel eikonal approximation is clearly invalid for backward scattering, calculations were nevertheless performed in the full angular range $0 \leq \theta \leq 180^\circ$ so as to illustrate certain inadequacies of the treatment. Its failure to properly describe large angle scattering in figures 5 and 6 is a direct result of the explicit neglect of electron-exchange - some of which, however, is implicitly included by virtue of the multistate expansion - and by the adoption of a straight line trajectory so as to ease computation of both the eikonal (or phase-distortion to the relative motion) in each channel and of the transition amplitudes C_n coupling the various channels. The Glauber and Born approaches also suffer from

these defects. These effects, however, can be incorporated directly within the basic eikonal model, although a combination of a full quantal partial-wave analysis of the close encounters responsible for these effects and a multichannel eikonal method for the more distant encounters is perhaps a better alternative.

Although electron-exchange is needed to reproduce inelastic scattering by $\theta \geq 50^\circ$, the contribution arising from these larger scattering angles to the total excitation cross section is however extremely small.

3.3 λ, χ and orientation parameters

In figures 7 and 8 the present predictions of $\lambda(2^1P)$ and $\lambda(3^1P)$ obtained from eq. (3), are compared with the measurements of Eminyan et al. (1974, 1975) and with the available distorted wave and many-body calculations. Agreement with experiment is good, particularly at the smaller scattering angles. Measurements however are not available for scattering by $\theta \leq 15^\circ$, an angular region for which the present multichannel eikonal treatment is particularly successful (cf. figures 5 and 6). It is also worth noting that the goodness of the many-body treatment of the 2^1P total and differential excitation (cf. figures 2 and 6) is not maintained for $\lambda(2^1P)$ at the larger scattering angles. After the present λ -curves reach their minima at angles θ which decrease with increasing E , they tend monotonically toward unity as $\theta \rightarrow 180^\circ$.

The present variation of λ with E and θ is presented in figure 9. Since λ denotes the relative contribution arising from the $M = 0$ sublevel to the 2^1P differential cross section, figure 9 shows quite clearly that for scattering through $\theta \leq 20^\circ$, excitation of the $M = \pm 1$ substates dominates with increasing E , except in the near vicinity of the forward direction $\theta = 0$ when only $\Delta M = 0$ transitions occur. The small-angle region $\theta \leq 20^\circ$ contributes

most to the total cross section which is therefore primarily controlled by the $M = \pm 1$ excitations at high impact energies (cf. table 1). For scattering through larger angles (past the λ -minima), the trend is reversed with excitation of the $M = 0$ sublevel dominating at high E , although here, its relative contribution to the total cross section is negligible.

The parameter $|\chi|$ which is a measure of the coherence between the excitations of the $M = 0$ and ± 1 sublevels (or phase difference between the corresponding oscillating and rotating dipoles, respectively) is displayed in figures 10 and 11 for transitions to the 2^1P and 3^1P levels. The 2^1P -measurements are bracketed by the distorted-wave and the present ten channel-eikonal results. The weak structure in $\chi(3^1P)$ is reproduced, although at somewhat larger angles.

The variation of χ (which is negative) with θ and E is displayed in figure 12. For high E and small θ , χ tends to zero in harmony with the prediction of Born's approximation, although for intermediate energies $E \leq 100$ eV, a non-zero limit is attained. When χ passes through $\frac{\pi}{2}$ i.e., when the phases of the oscillating and rotating dipoles differ by $\frac{\pi}{2}$, and, provided that the magnitudes of the corresponding amplitudes are about equal (i.e., $\lambda \approx 0.5$), then at this particular scattering angle θ_c , full circularly polarized light would be observed in a direction at right-angles to the plane of scattering.

The departure from equal population of the $M = 0$ and ± 1 states at θ_c is obtained from figure 9 and hence circularly polarized light will be observed for scattering angles whose shift from θ_c depends on the function $\lambda(\theta)$. The fraction Π of circularly polarized radiation emitted perpendicular to the XZ-plane of scattering is the following combination

$$\Pi(\theta, E) = - 2[\lambda(1 - \lambda)]^{\frac{1}{2}} \sin \chi \quad (23)$$

of λ and χ . Figure 13 displays the present variation of Π with θ and E .

Fully circular-polarized light (i.e. $\Pi = 1$) is in evidence only for low energy, large-angle collisions. For scattering in the forward direction, Π is small and almost independent of E . The recognition that Π is also $\overline{\Delta L}_Y$, the angular momentum transferred in a direction Y perpendicular to the assumed XY -plane or scattering provides some further insight to figure 13. In the impulsive high-energy limit, the torque \underline{N} about an origin O due to a force \underline{F} acting on an electron at position vector $\underline{r}(x, y, z)$ for time Δt is, from classical mechanics,

$$\underline{N} = \underline{r} \times \underline{F} = \frac{\Delta \underline{L}}{\Delta t} \quad (24)$$

and hence the Y -component to the change ΔL in angular momentum is

$$\Delta L_Y = [\langle \underline{r} \rangle \times \Delta \underline{P}]_Y = 2 k_i \sin \frac{\theta}{2} \langle z \rangle \quad (25)$$

where $\Delta \underline{P}$ is the linear momentum $2k_i \sin \frac{\theta}{2}$ transferred and $\langle \underline{r} \rangle$ is some time average of \underline{r} during the impulsive encounter. Small-angle collisions with an atom result from distant encounters, and the target atom and hence $\langle z \rangle$ remains essentially unaffected. Thus $\overline{\Delta L}_Y$ increases as $E^{\frac{1}{2}}$ and θ , until sufficiently large E and θ when large-angle, close-encounter collisions dominate such that the expectation value $\langle z \rangle$ must decrease more rapidly than $E^{\frac{1}{2}} \sin \frac{\theta}{2}$ so as to cause the decreasing $\overline{\Delta L}_Y$ observed in figure 13.

In conclusion, the present version of the multichannel eikonal treatment provides a successful description of inelastic collisions at intermediate and high impact-energies. Its success for total excitation cross sections can be attributed to the fact that here the small-angle scattering ($\theta \leq 50^\circ$) which dominates the total cross section even at low energies ($E \approx 40$ eV) is well described. The main effects, such as intermediate (long-range) couplings between each channel, some polarization of each target state, and static-

distortion in each channel needed for a correct description of small-angle scattering are included. Also the multichannel eikonal expansion ensures (a) that convergence in partial wave contributions is always attained especially in the high-energy limit (b) that the long-range couplings can effect distant encounters (or large total angular momentum), and also (c) that some account of electron-exchange is provided. More basic parameters such as λ (which yields the relative contribution of the $M = 0$ excitation to the differential cross section) and χ (which is the phase difference between the $M = 0$ and ± 1 scattering amplitudes) are also well described as functions of E and θ , particularly at the smaller scattering angles. In order to properly describe large-angle inelastic scattering, the present version of this treatment would however require modification so as to explicitly include effects arising from electron-exchange and orbit-distortion.

Acknowledgment

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Table 1: Total excitation cross sections $Q(10^{-2} \pi a_0^2)$ given by a ten-channel treatment of the processes
 $e + \text{He}(1^1\text{S}) \rightarrow e + \text{He}(n^1\text{L})$
at incident-electron energies $E(\text{eV})$.

$E(\text{eV}) \backslash nL$	2^1S	2^1P_0	$2^1\text{P}_{\pm 1}$	2^1P	3^1S	3^1P_0	$3^1\text{P}_{\pm 1}$	3^1P	3^1D_0	$3^1\text{D}_{\pm 1}$	$3^1\text{D}_{\pm 2}$	3^1D
40	2.45	6.92	4.86	11.78	$2.89^{-1\dagger}$	1.83	0.85	2.68	1.11^{-1}	1.12^{-1}	2.46^{-2}	2.48^{-1}
50	2.27	6.95	6.09	13.04	2.93^{-1}	1.89	1.15	3.04	8.38^{-2}	9.55^{-2}	2.95^{-2}	2.09^{-1}
60	2.12	6.77	6.89	13.66	3.02^{-1}	1.86	1.38	3.24	6.92^{-2}	8.04^{-2}	3.24^{-2}	1.82^{-1}
80	1.84	6.18	7.50	13.68	2.86^{-1}	1.65	1.60	3.25	4.70^{-2}	5.75^{-2}	3.39^{-2}	1.38^{-1}
100	1.61	5.52	7.60	13.12	2.69^{-1}	1.48	1.69	3.17	3.56^{-2}	4.31^{-2}	3.36^{-2}	1.12^{-1}
150	1.22	4.34	7.22	11.56	2.18^{-1}	1.12	1.69	2.81	2.10^{-2}	2.63^{-2}	3.01^{-2}	7.74^{-2}
200	9.86^{-1}	3.54	6.67	10.21	1.84^{-1}	8.96^{-1}	1.60	2.50	1.50^{-2}	1.85^{-2}	2.66^{-2}	6.01^{-2}
300	7.07^{-1}	2.50	5.69	8.19	1.40^{-1}	6.22^{-1}	1.40	2.02	9.40^{-3}	1.08^{-2}	2.13^{-2}	4.15^{-2}
400	5.49^{-1}	1.81	5.02	6.83	1.12^{-1}	4.49^{-1}	1.25	1.70	6.83^{-3}	7.35^{-3}	1.77^{-2}	3.19^{-2}
500	4.49^{-1}	1.31	4.54	5.85	9.24^{-2}	3.30^{-1}	1.13	1.46	5.52^{-3}	5.39^{-3}	1.52^{-2}	2.61^{-2}
500*	4.46^{-1}	1.20	4.66	5.86	8.71^{-2}	3.12^{-1}	1.15	1.46	-	-	-	-
500†	4.84	-	-	6.02	1.09^{-2}	-	-	1.49	-	-	-	2.51^{-2}

† Superscript denotes the power of 10 by which the entry must be multiplied.

* Four-channel treatment (1^1S $n^1\text{S}$ $n^1\text{P}_{0,\pm 1}$)

† Born (Bell et al. 1969)

Table 2: Polarization Fractions of the Radiation Emitted from $\text{He}(n^1\text{L})$

$E(\text{eV}) \backslash n^1\text{L}$	2^1P	3^1P	3^1D
40	.480	.624	.377
50	.391	.533	.327
60	.326	.459	.287
80	.245	.347	.211
100	.185	.273	.149
150	.092	.140	.039
200	.030	.057	-.030
300	-.065	-.059	-.122
400	-.162	-.164	-.179
500	-.268	-.263	-.215

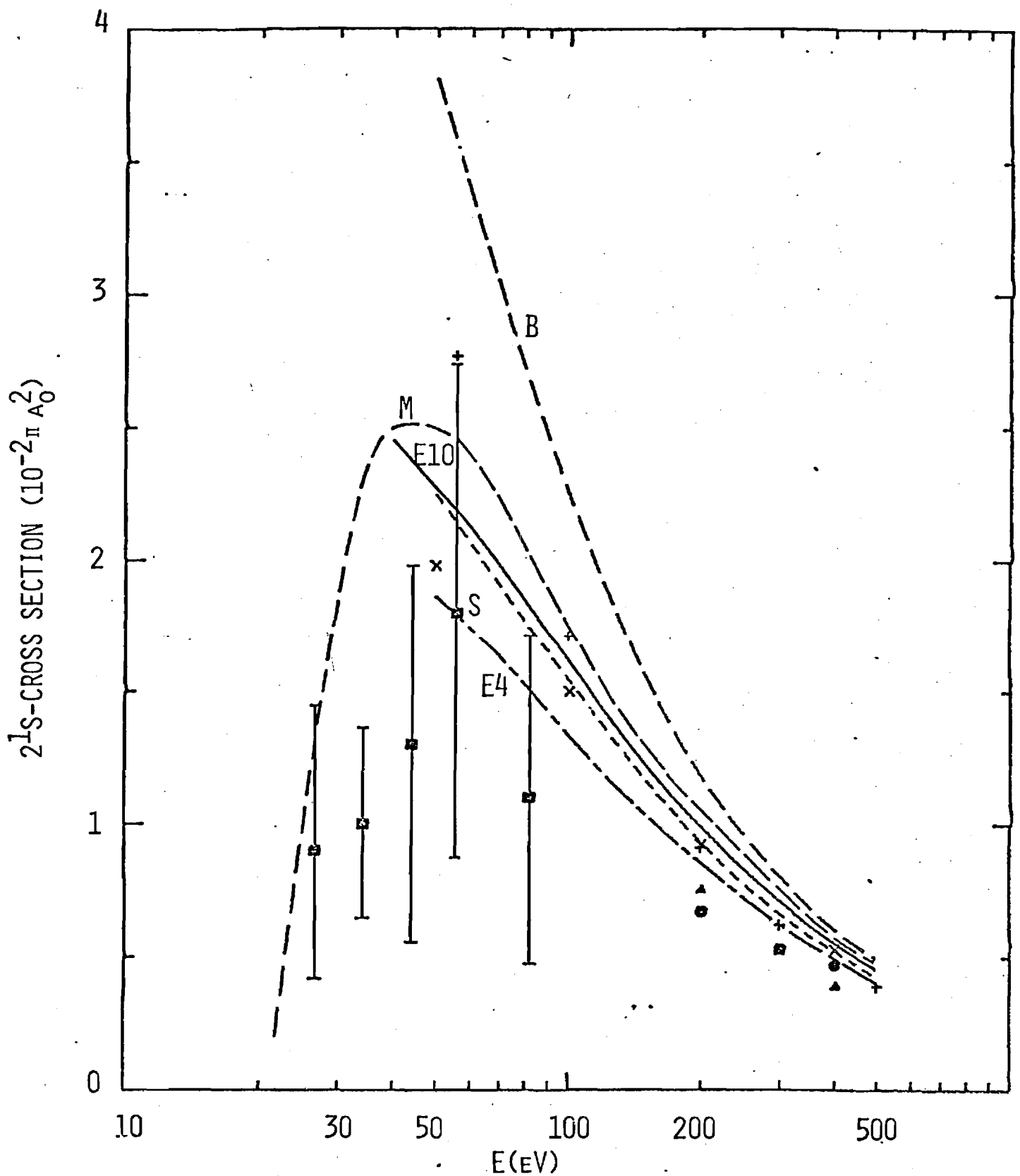


Figure 1: Total cross section for the $1^1S - 2^1S$ transition in He by collision with electrons of energy E (eV). Theory: E4, E10, present ten- and four-channel eikonal treatments, respectively. S; second-order potential method with simple set of wavefunctions (Berrington et al. 1973). M; first-order many-body approach (Thomas et al. 1974). B; Born Approximation (Bell et al. 1969). X; second-order diagonalization method (Baye and Heenen 1974). +; Glauber Approximation (Chan and Chen 1973, 1974a). Experiment: \square ; Rice et al. (1972). \triangle ; Miller et al. (1969). \bullet ; Vriens et al. (1968).

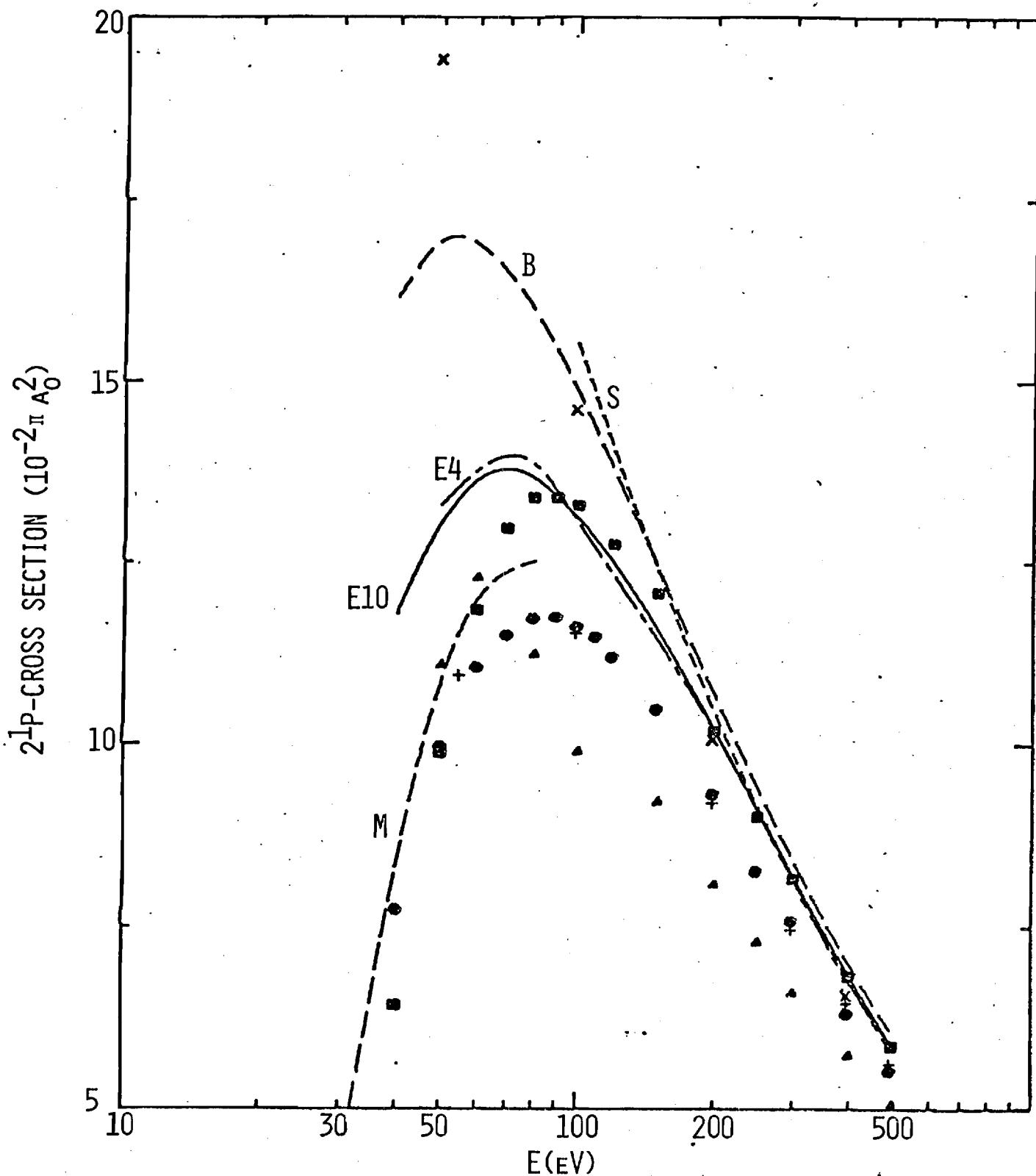


Figure 2: Total cross section for the $1^1S - 2^1P$ transition in He by collision with electrons of energy E (eV). Theory: Exactly as in figure 1. Experiment: ● ; Donaldson et al. (1972). ■ ; de Jongh and van Eck (1971). ▲ ; Moustafa Moussa et al. (1969).

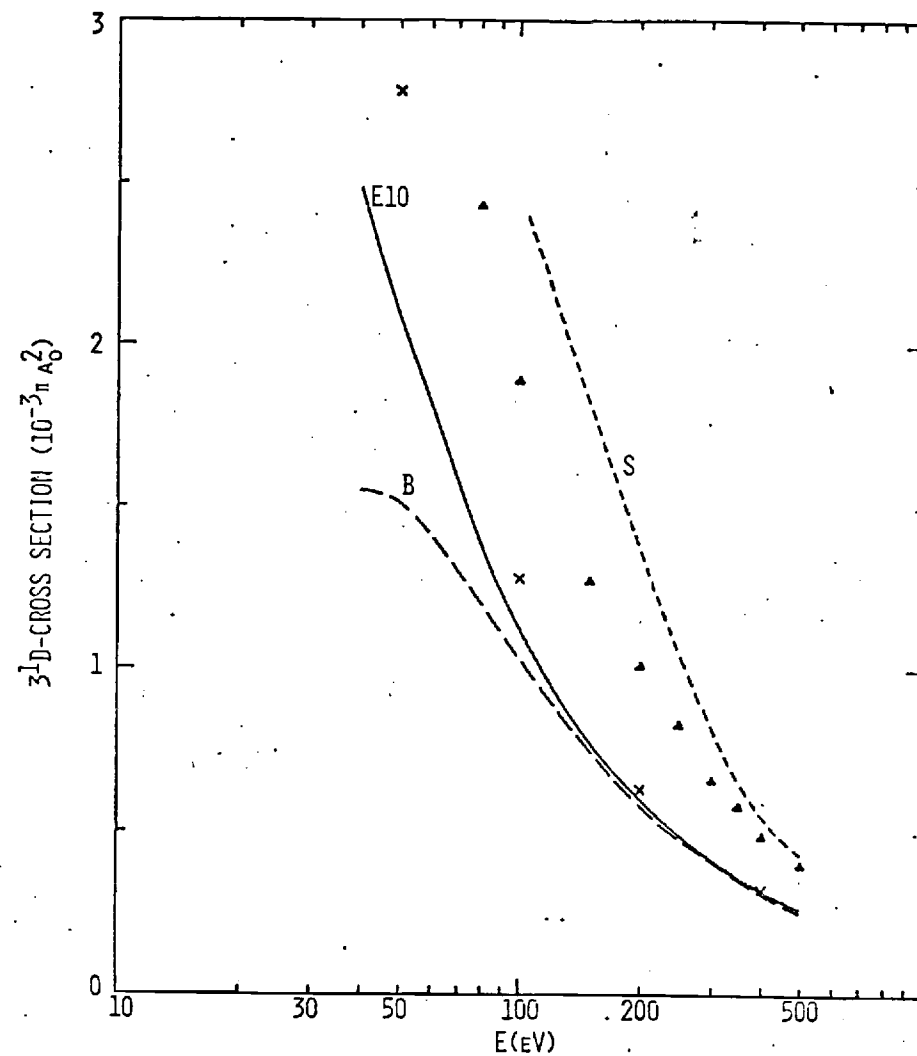
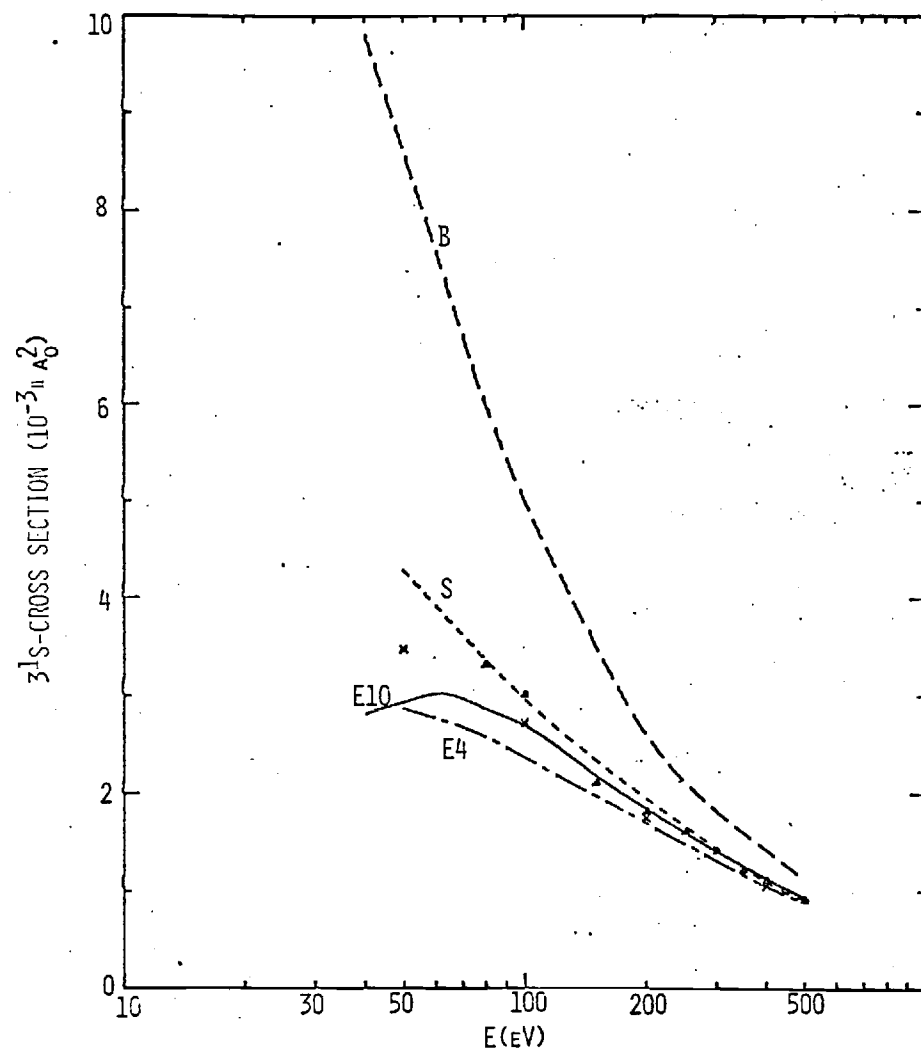


Figure 3: Total cross section for excitation of (a) the 3^1S and (b) the 3^1D states of He by collision with electrons of energy $E(\text{eV})$. Theory: as in figure 1 except S; Second-order potential method (Bransden and Issa 1975). Experiment: \blacktriangle ; Moustafa Moussa et al. (1969).

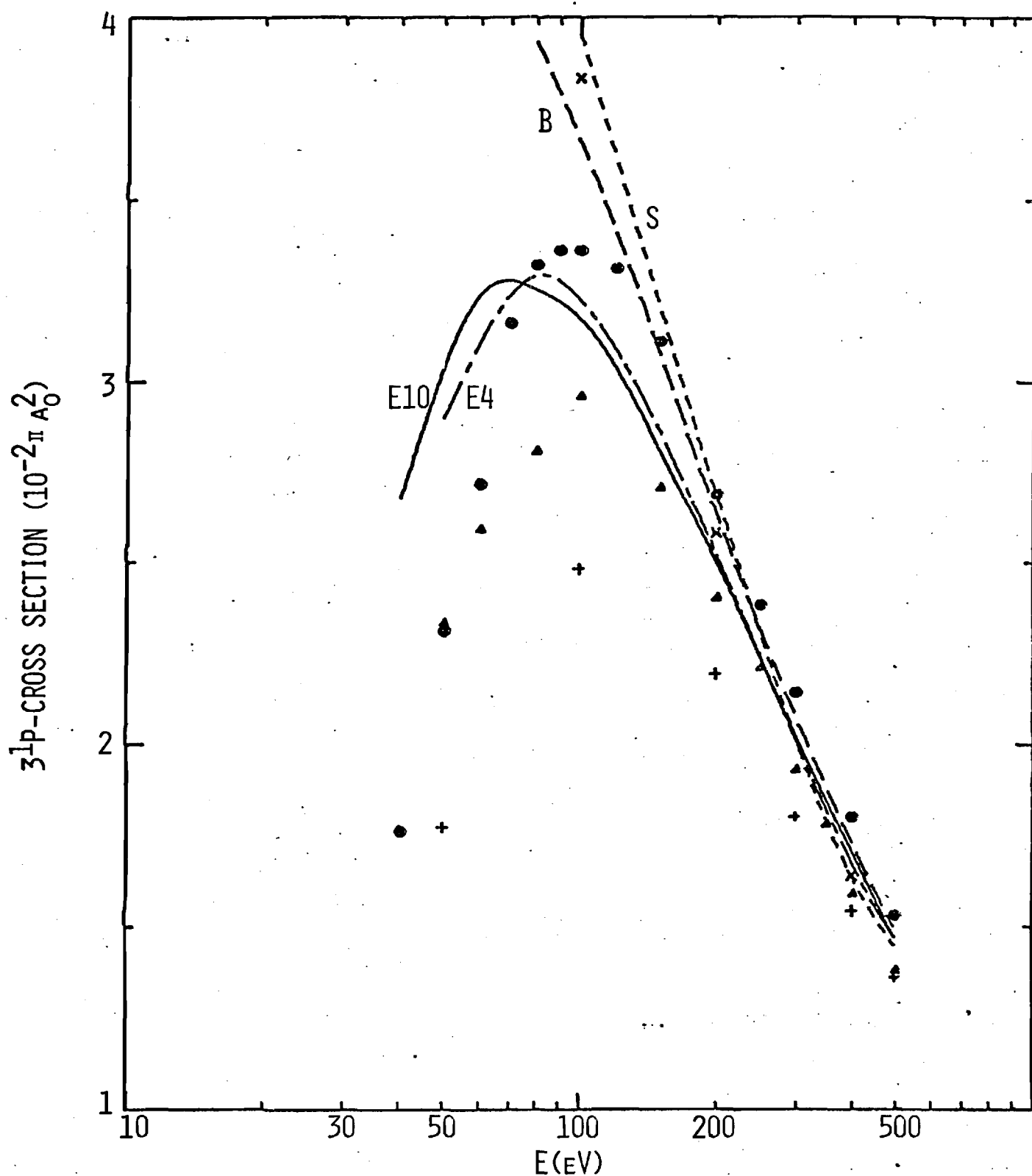


Figure 4: Total cross section for the $1^1S - 3^1P$ transition in He by collision with electrons of energy E (eV). As in figure 3.

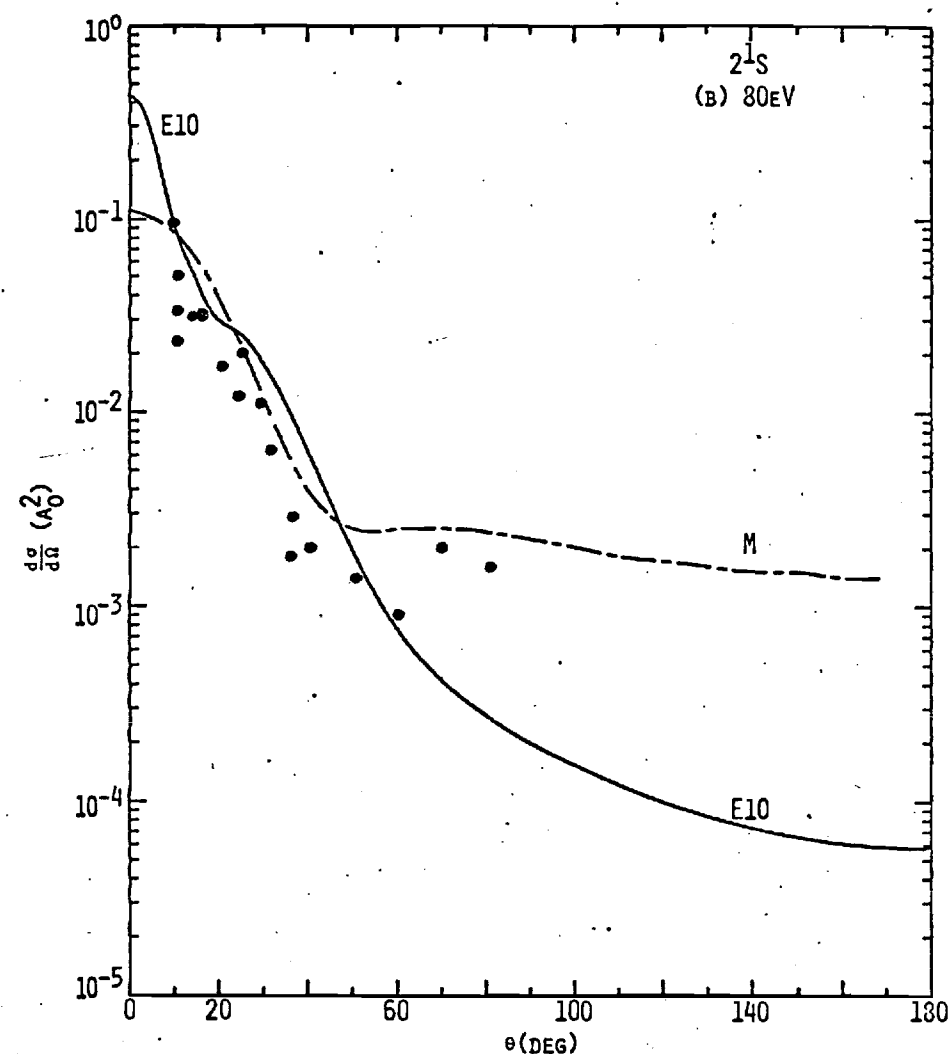
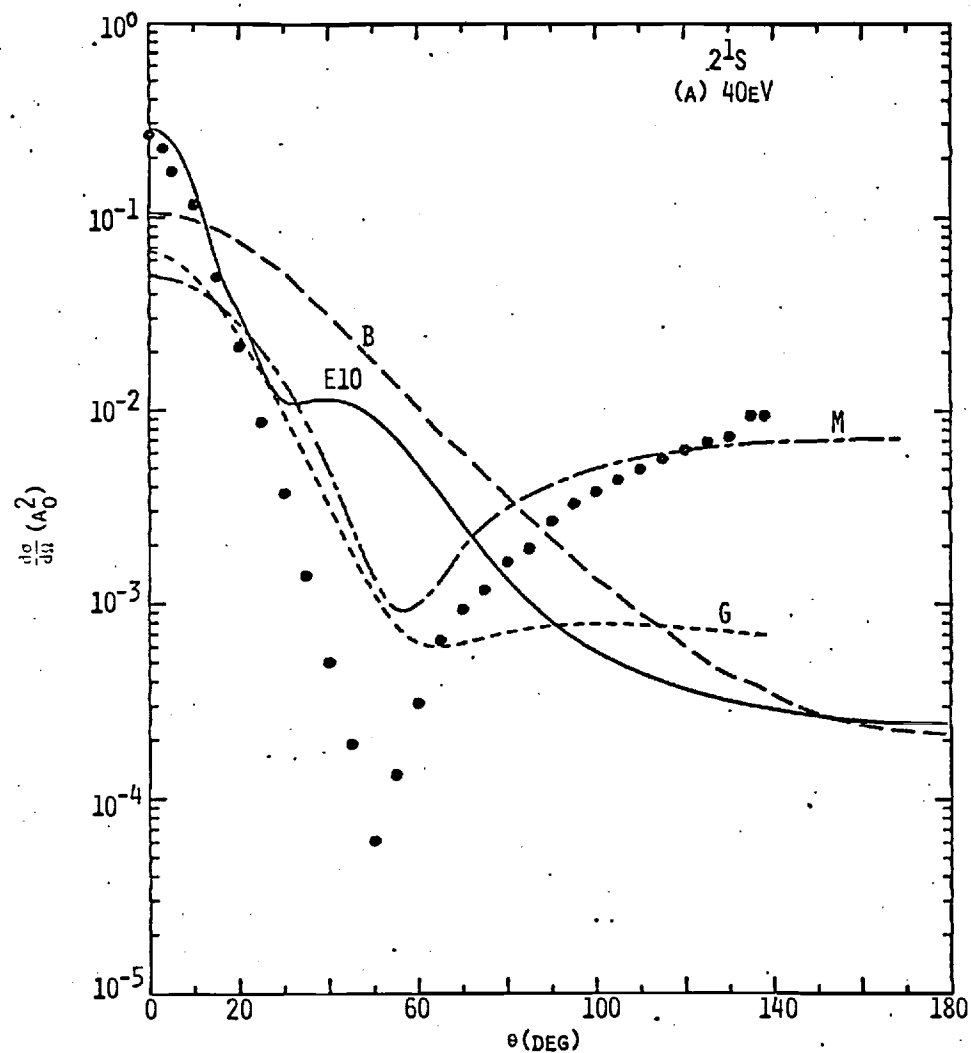


Figure 5: Differential cross sections for the 2¹S excitation of He by electrons with energy (a) 40 eV and (b) 80 eV. Theory: E10; present ten-channel eikonal treatment. M; first-order many-body approach (Thomas et al. 1974). G; B; Glauber and Born Approximations (see Trajmar (1972)). Experiment: ● ; (a) Trajmar (1973), (b) Rice et al. (1972).

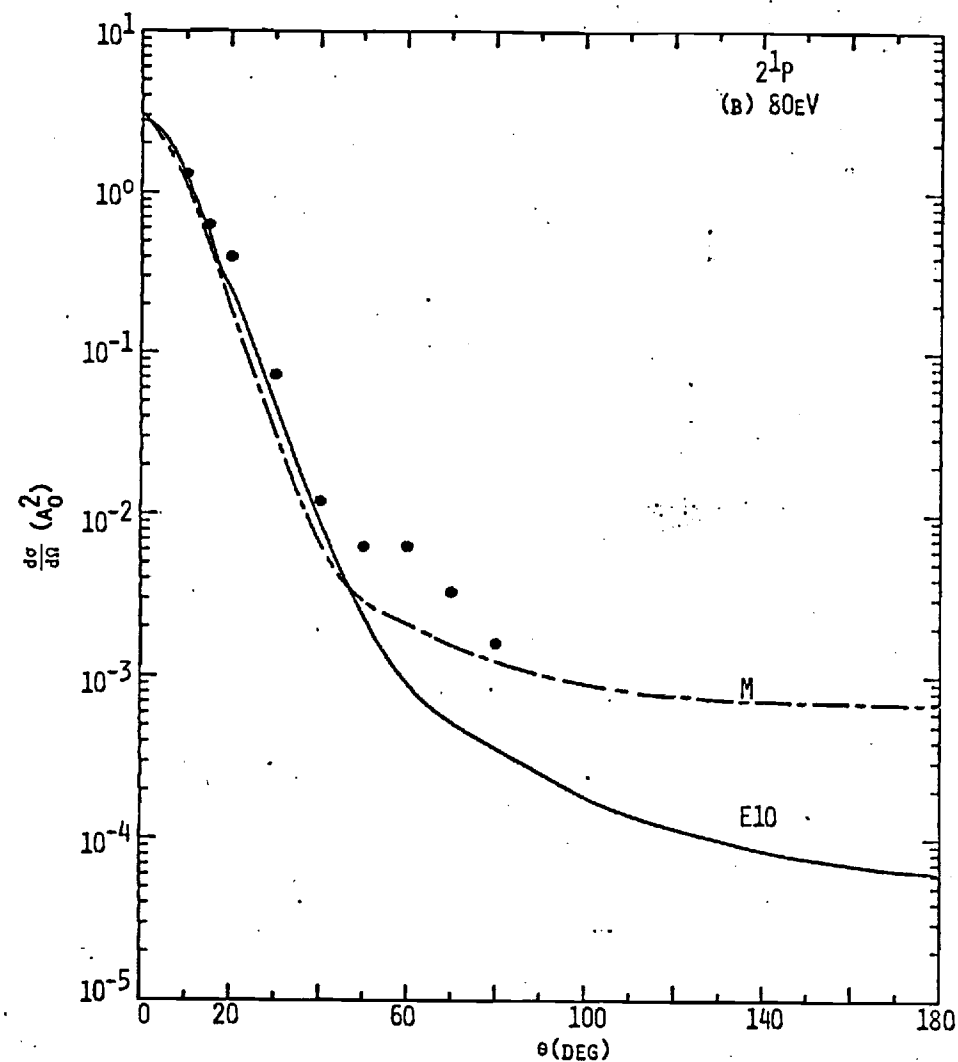
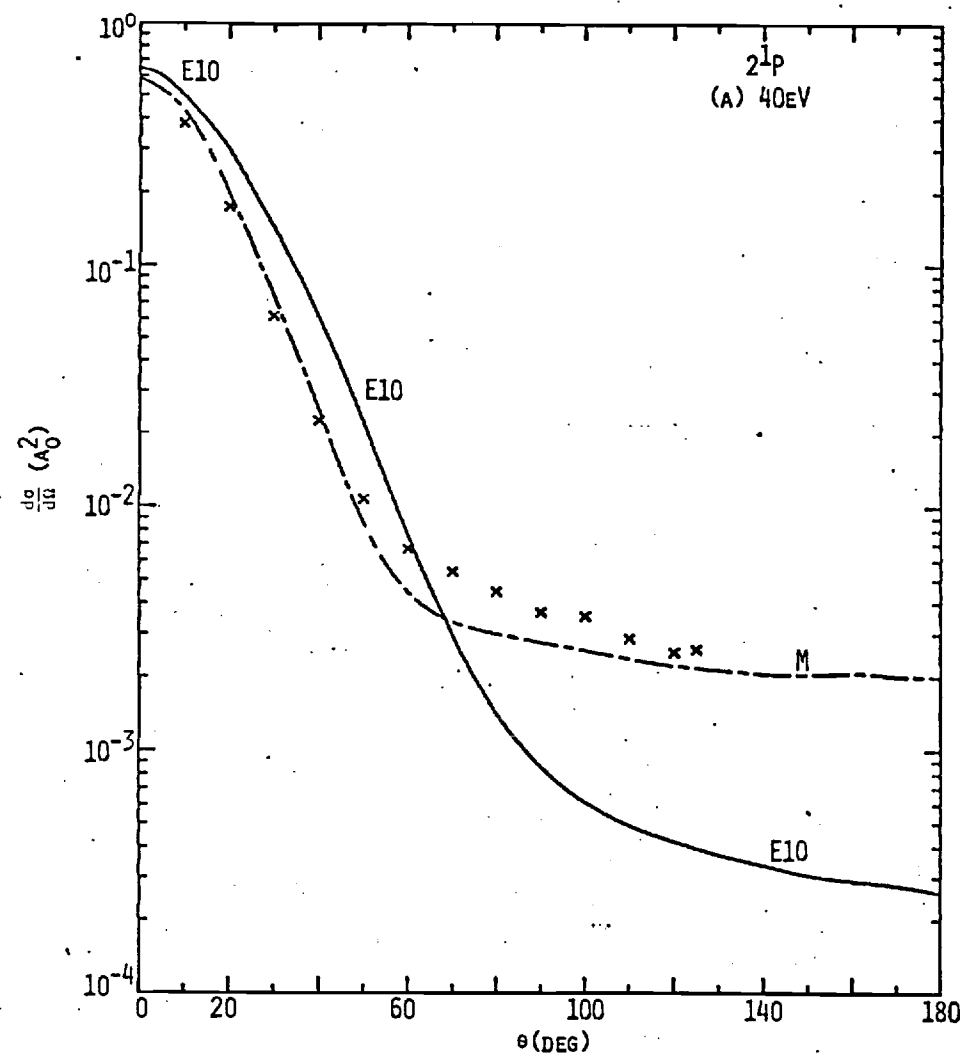


Figure 6: Differential cross sections for the 2^1P excitation of He by electrons with energy (a) 40 eV and (b) 80 eV. Theory: as in figure 5. Experiment: X; Hall et al. (1973). ● Truhlar et al. (1970).

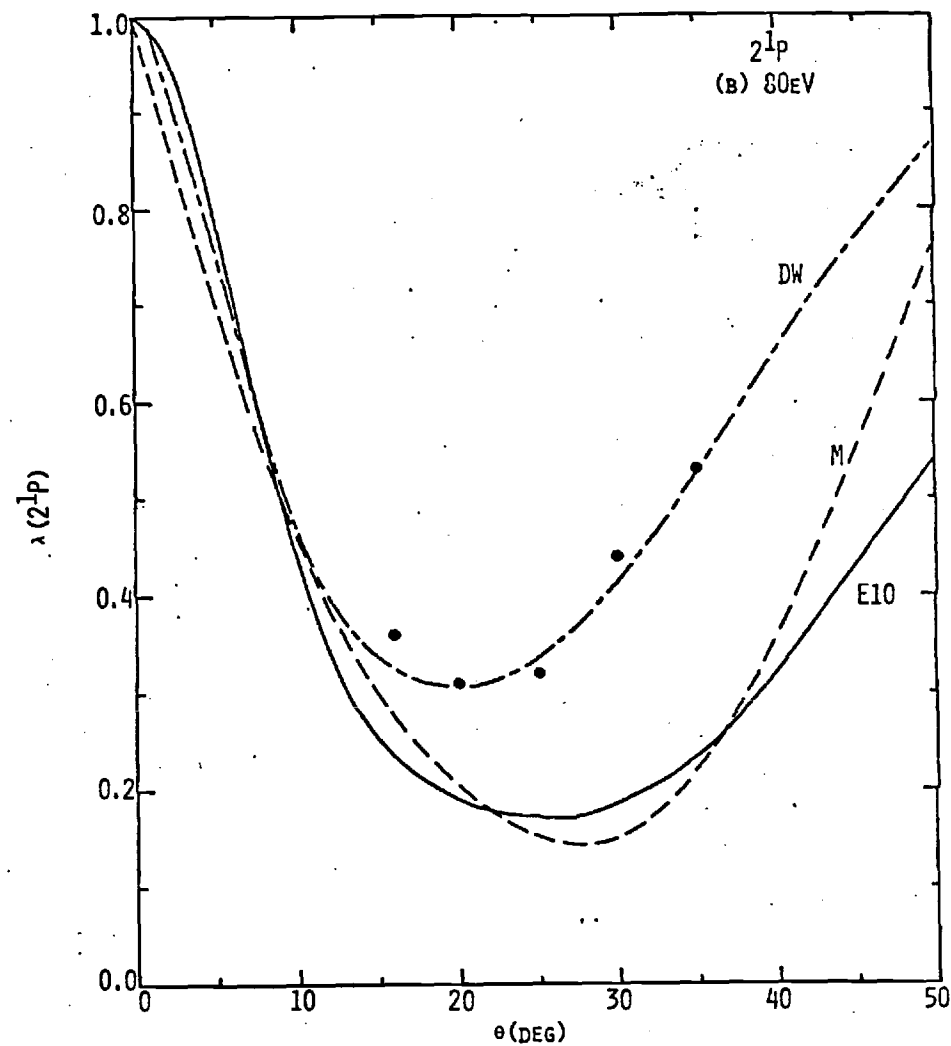
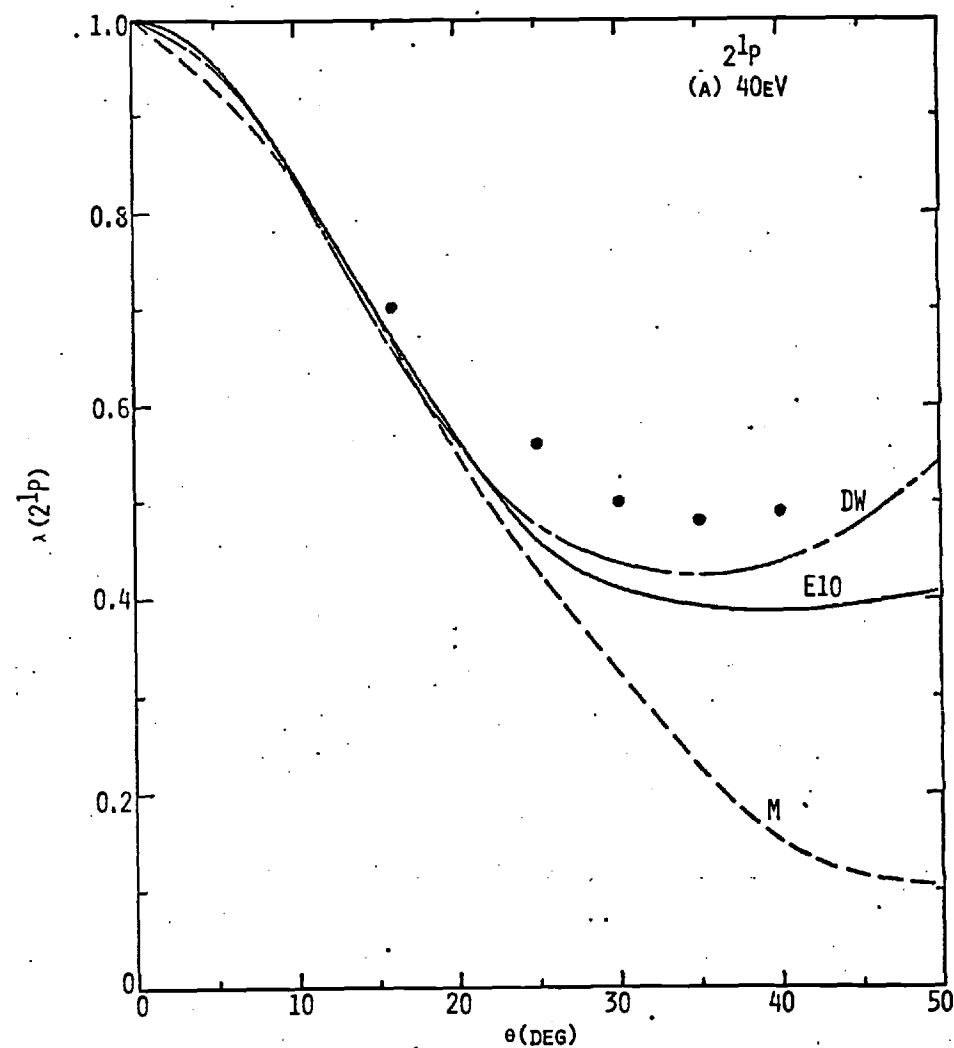


Figure 7: Variation of $\lambda(2^1P)$ with scattering angle θ at impact-energies (a) 40 eV and (b) 80 eV. E10; present ten-channel treatment. DW; Distorted-wave Born Approximation (Madison and Sheldon 1973). M; First-order many-body approach (Thomas et al. 1974). ● ; Eminyan et al. (1974).

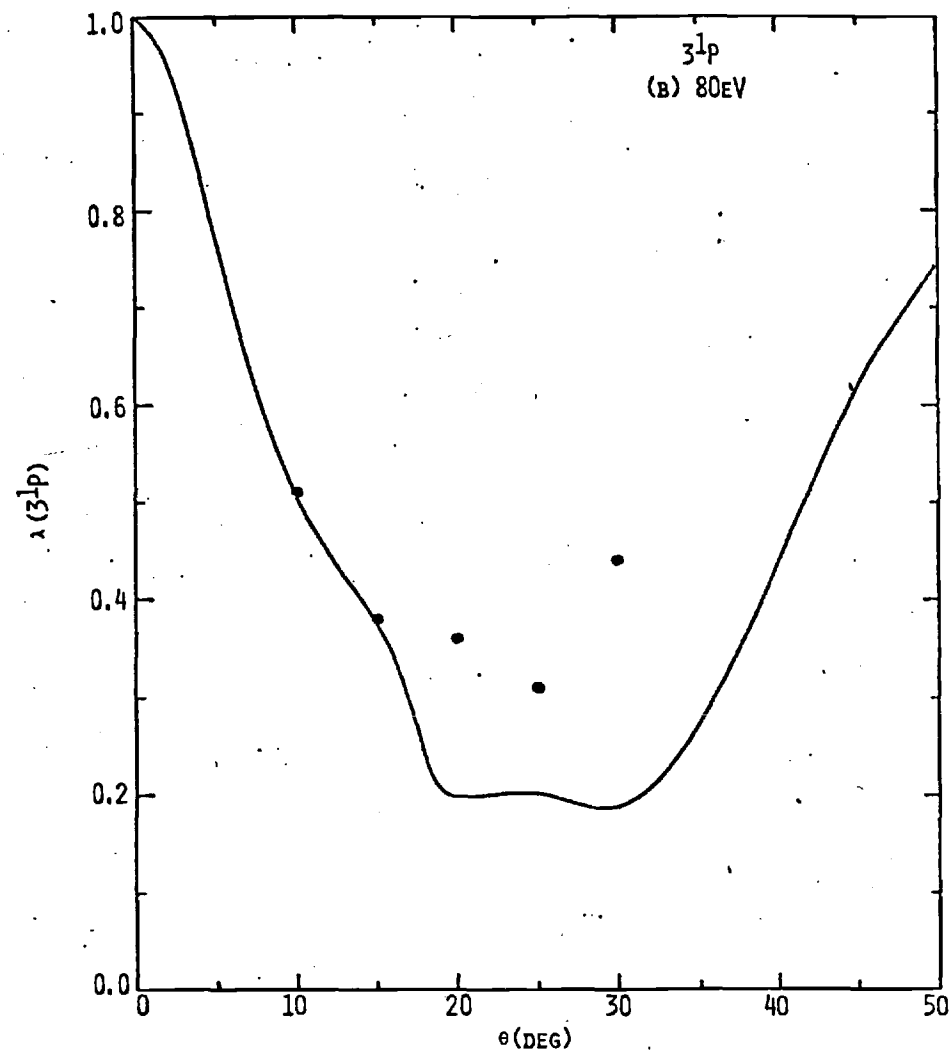
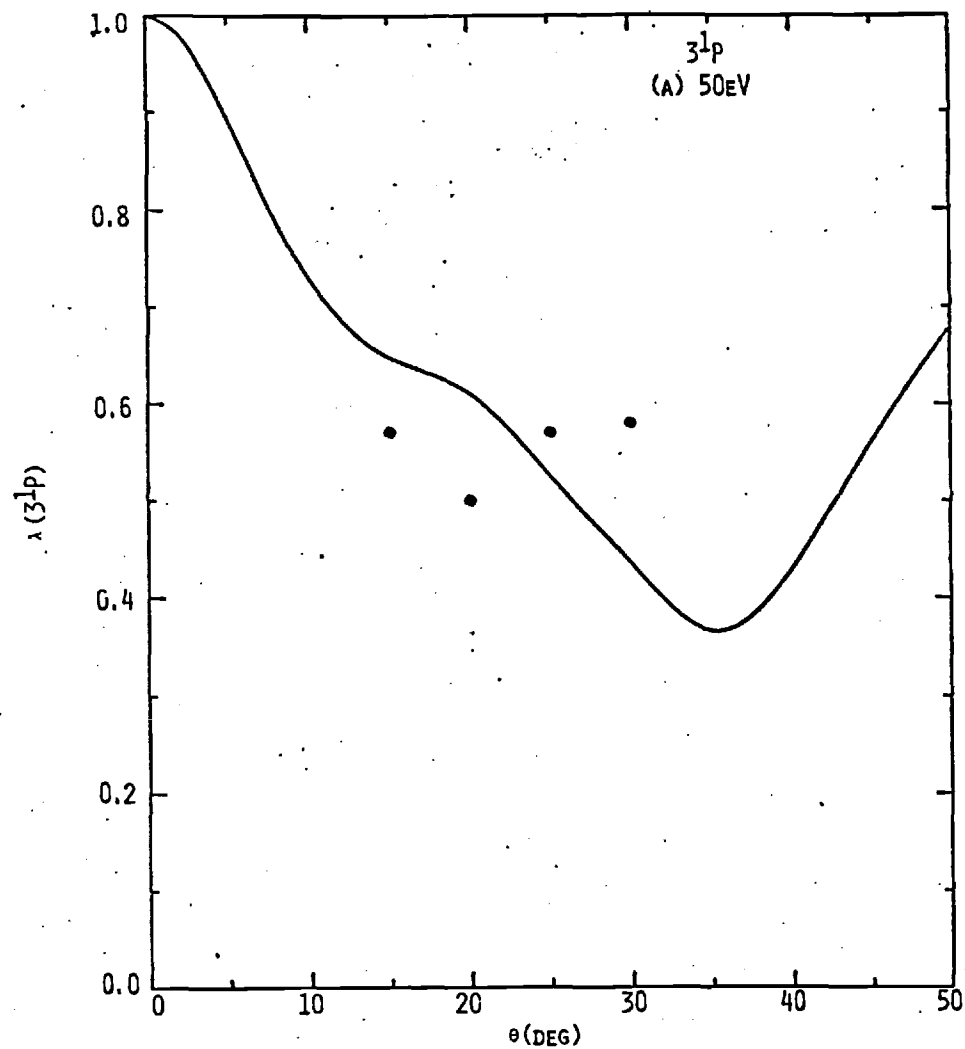


Figure 8: Variation of $\lambda(3^1P)$ with scattering angle θ at impact-energies (a) 50 eV and (b) 80 eV. E10; present ten-channel treatment.
 ● ; Eminyan et al. (1975).

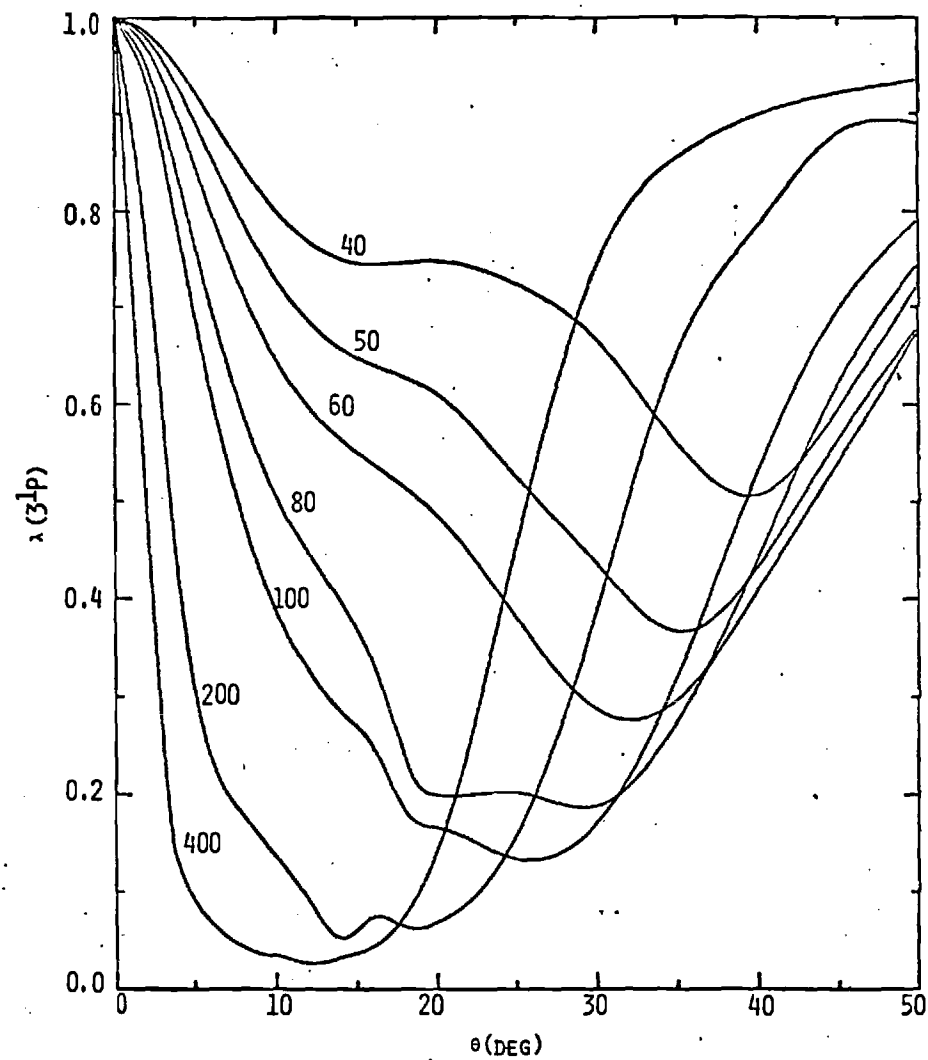
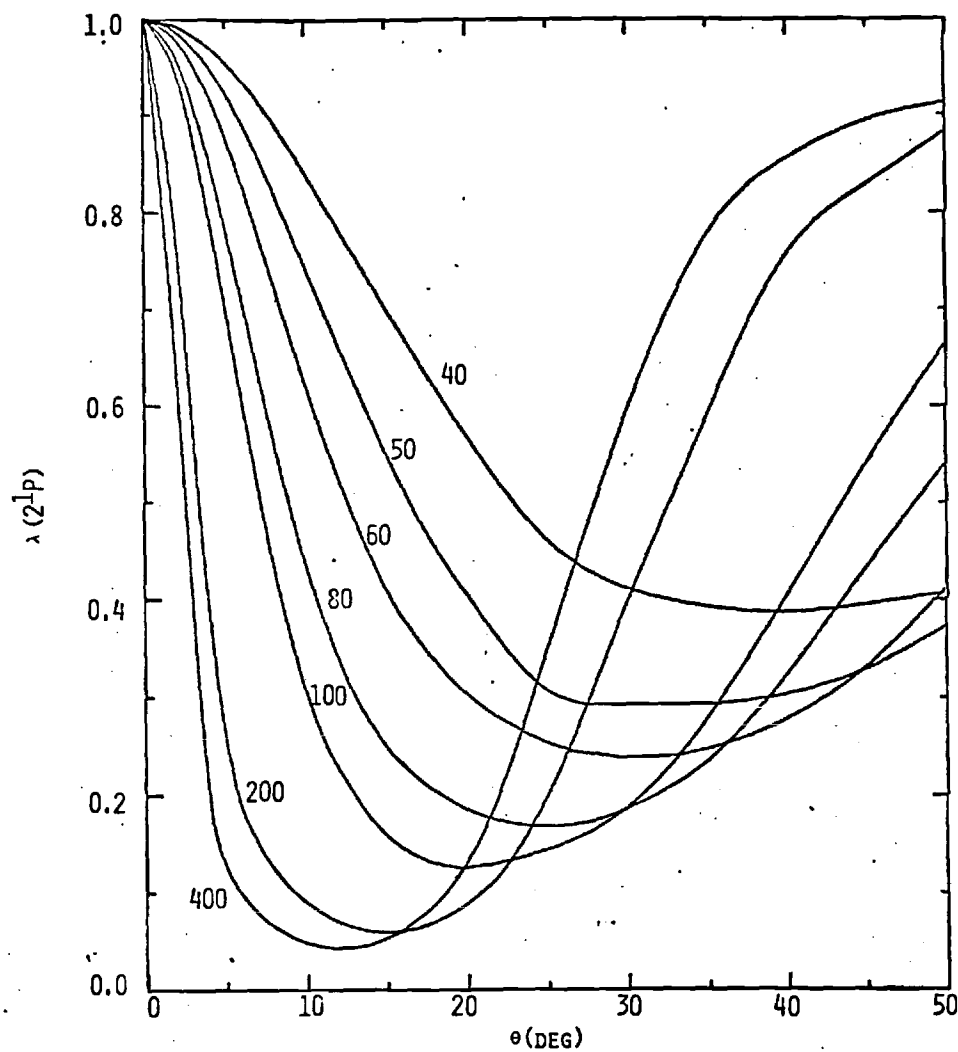


Figure 9: Present variation of (a) $\lambda(2^1P)$ and (b) $\lambda(3^1P)$ with scattering angle θ° , and with impact-energy E (eV), indicated on each curve.

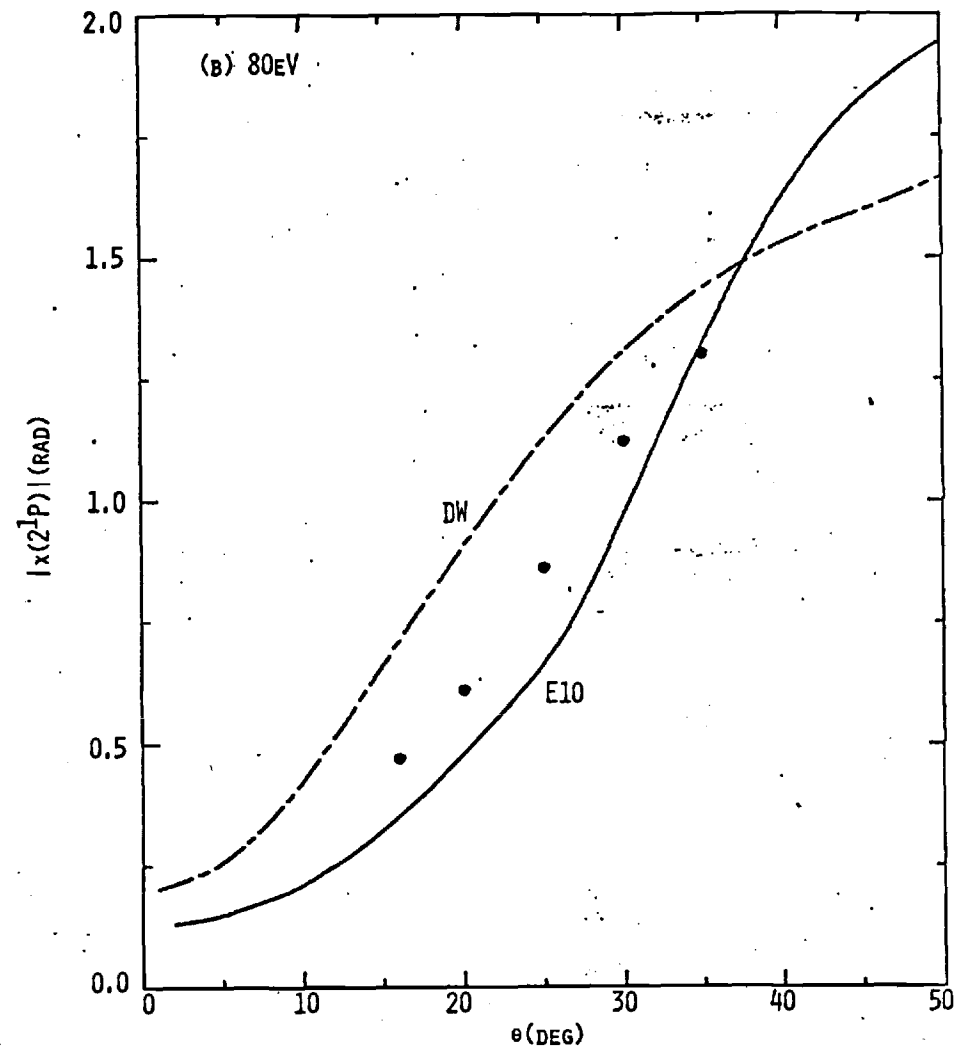
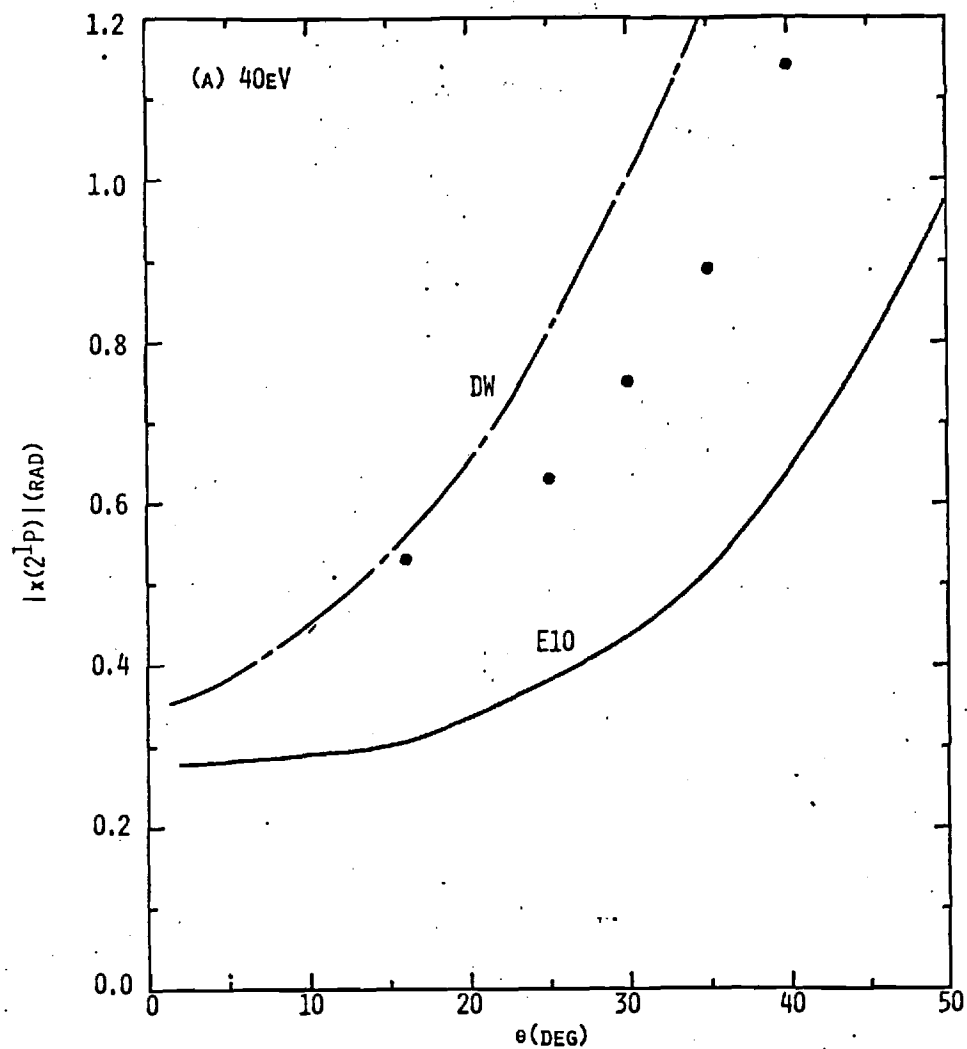


Figure 10: Variation of $|\chi(2^1P)|$ with scattering angle θ° at impact-energies (a) 40 eV and (b) 80 eV. E10; present ten-channel treatment. DW; Distorted-wave Born Approximation (Madison and Shelton 1973). \bullet ; Eminyan et al. (1974).

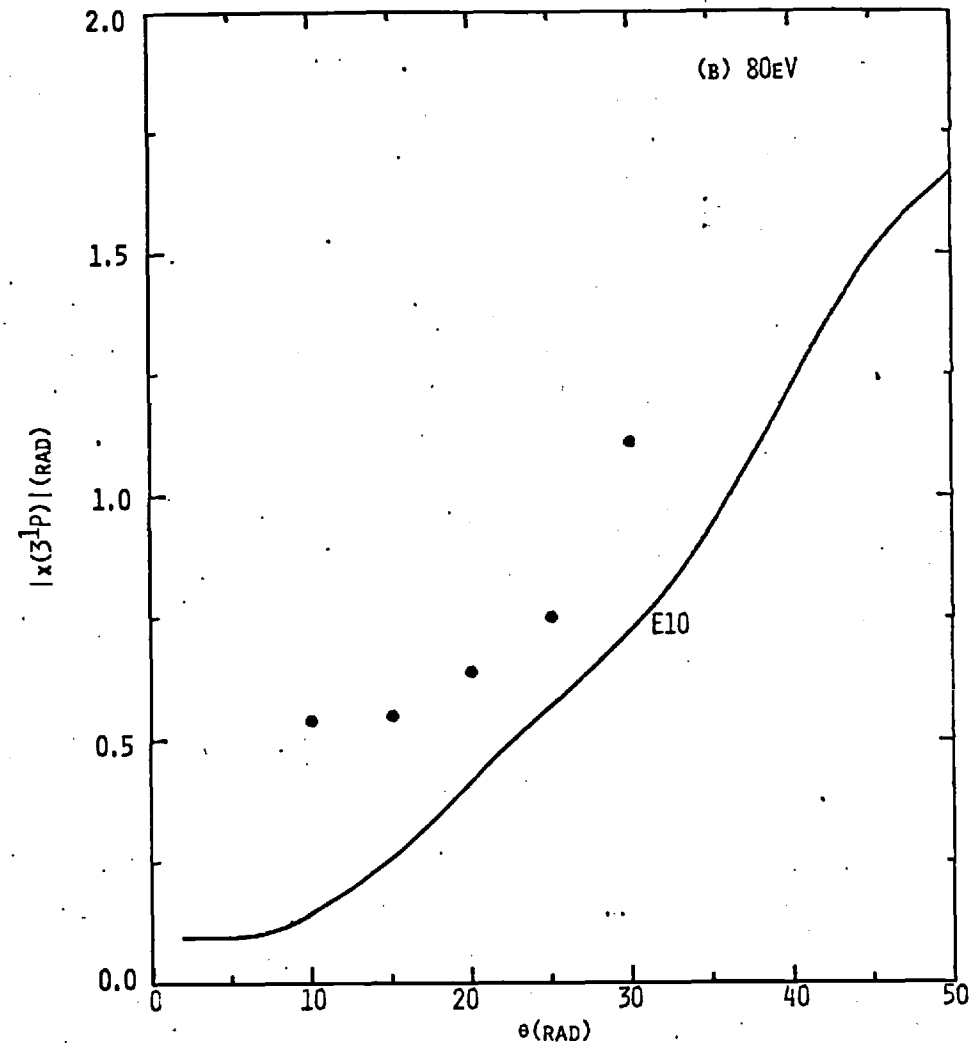
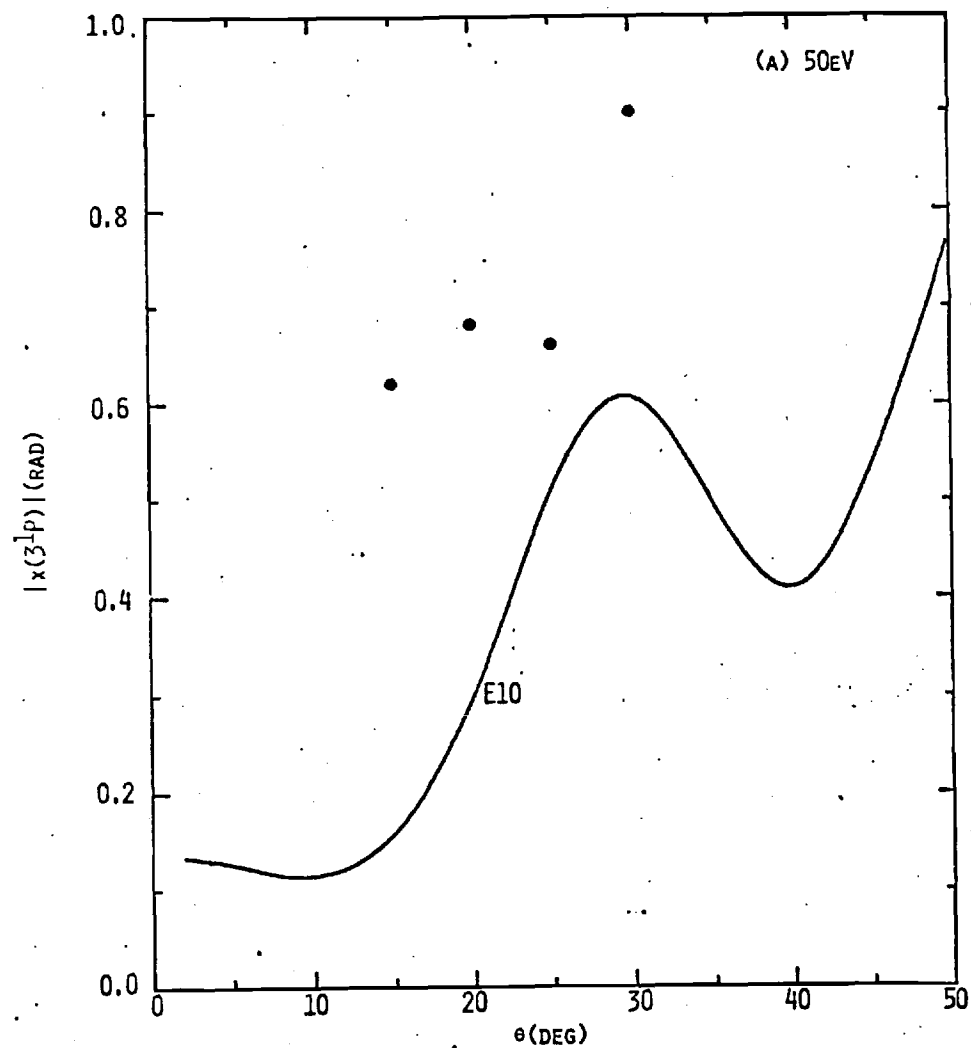


Figure 11: Variation of $|\chi(3^1P)|$ with scattering angle θ° at impact-energies (a) 50 eV and (b) 80 eV. E10; present ten-channel treatment.
 ● ; Eminyan et al. (1975).

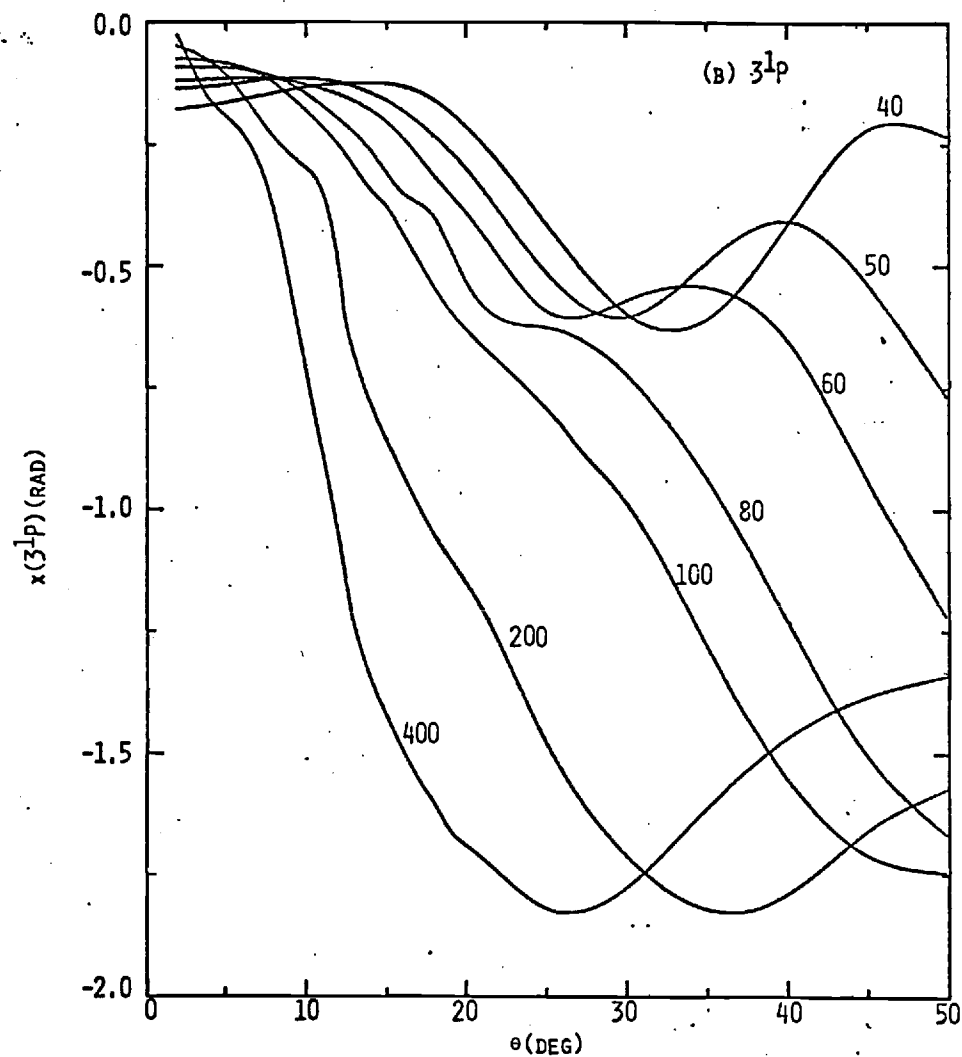
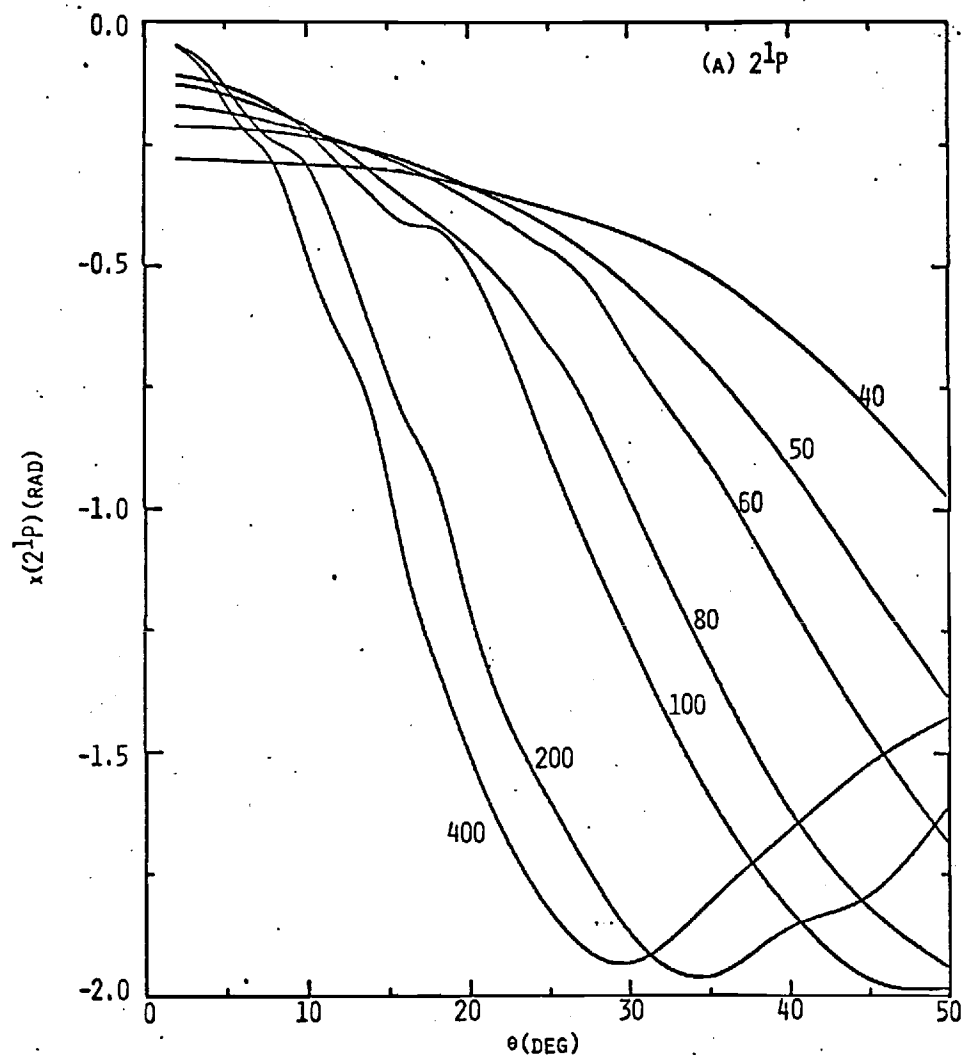


Figure 12: Present variation of (a) $\chi(2^1P)$ and (b) $\chi(3^1P)$ radians with scattering angle θ° and with impact-energy E (eV) indicated on each curve.

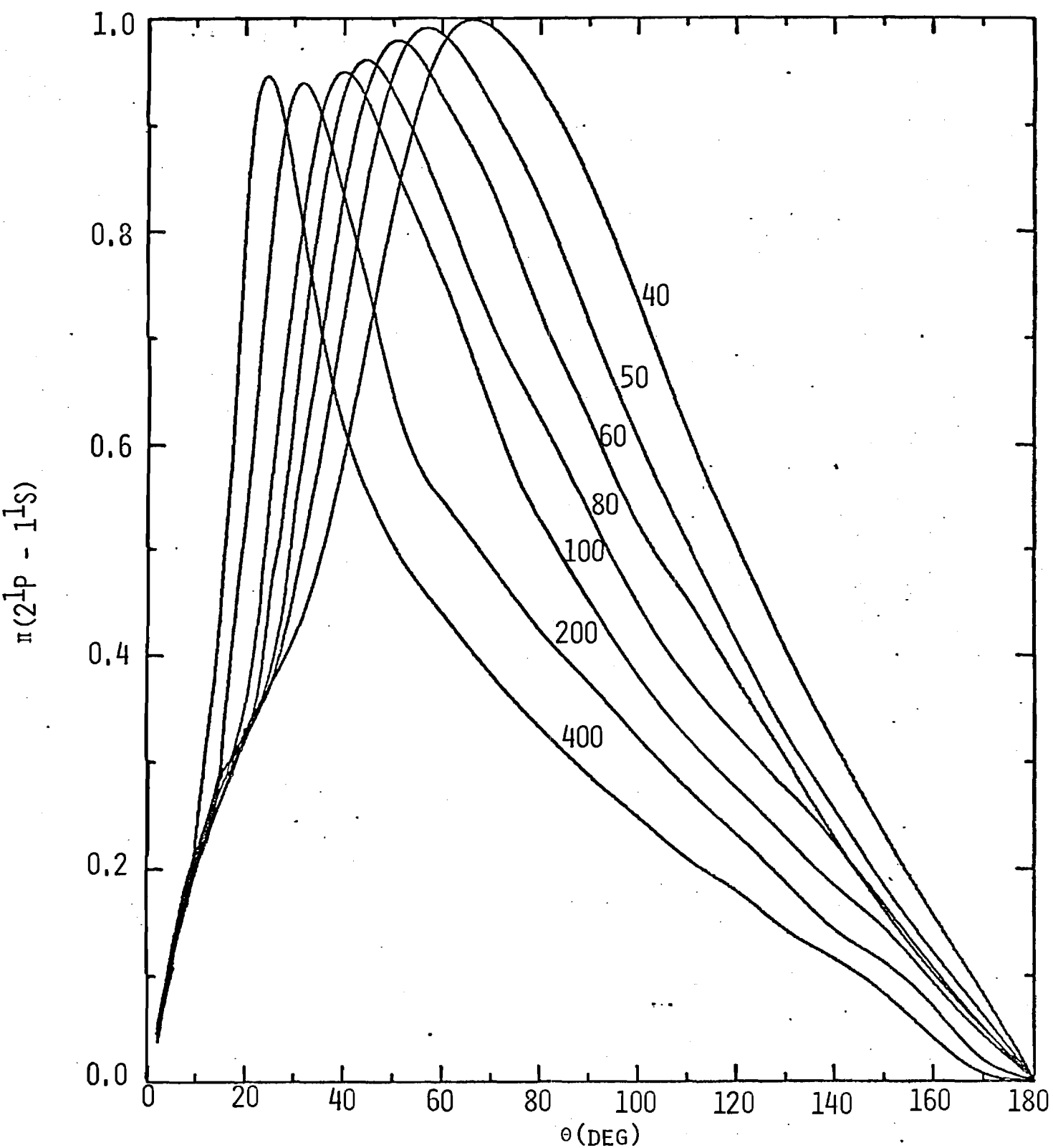


Figure 13: The variation of the fraction π of circularly polarized radiation, emitted from $\text{He}(2^1P)$ and observed at right-angles to the scattering plane, with scattering angle θ° and with impact-energy $E(\text{eV})$ indicated on each curve.

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GEORGIA INSTITUTE OF TECHNOLOGY

ATLANTA, GEORGIA 30332

April 8, 1975

SCHOOL OF PHYSICS

Air Force Aerospace Research Laboratories

ATTN: ARL/DO

Contract F33615-74-C-4003

Item No. 0002, Sequence No.

Wright-Patterson AFB, OH 45433

SUBJECT: Quarterly R and D Status Report No. 6
Principal Investigator, M. R. Flannery
covering the period 8 Jan., 75 - 8 April, 75

Gentlemen:

Transmitted herewith are four (4) copies of the subject report.

Should you have any questions or comments regarding this report,
please contact the principal investigator.

Sincerely,

M. R. Flannery

M.R. Flannery
Professor

MRF:jc
Enclosures

REPORT: Sixth Quarterly R & D Status Report
covering the period Jan. 8, 1975 - April 8, 1975

PROJECT-TITLE: Calculation of Electron Impact Cross Sections from
Metastable States in Atomic and Molecular Gases

PRINCIPAL INVESTIGATOR: M. R. Flannery
School of Physics
Georgia Institute of Technology
Atlanta, Georgia 30332

CONTRACT NO: F33615-74-C-4003

SPONSOR CONTACT PERSON: Lt. John F. Prince / Dr. Alan Garscadden
U. S. Air Force
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Bldg. 450, Area B
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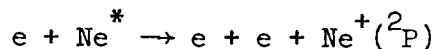
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Appendix B: Abstracts of papers submitted to IX ICPEAC	

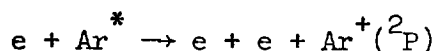
1. Progress achieved during the period 8 Jan. 1975 - 8 April 1975.

A thorough study of available methods suitable for the ionization problems was made.

(a) Total ionization cross sections for the processes involving metastable species (*),



and



were determined by the Born and the binary-encounter approximations. The calculation of the wavefunctions, form factors and the collision-integrals (four-dimensional) were extremely lengthy.

The resulting cross sections are displayed in figures 1 and 2 together with recent comparison values of Dixon, Harrison and Smith (private communication). The experiments are difficult and the amount of agreement is encouraging.

(b) A survey of methods applicable to ionization revealed that, apart from the simpler quantum-mechanical and binary-encounter descriptions, there are no treatments of ionization that are capable of systematic improvement (contrary to the case of excitation for which numerous methods based on close coupling exist). For ionization, the concept of close-coupling methods is alien to continuum states, a situation for which schemes need to be designed which are capable of systematic improvement. The problem is a difficult one. In appendix A of this report is included a theoretical treatment developed by M. R. Flannery and prepared for

submission for publication in J. Phys. B: Atom. Molec. Phys. The treatment represents a new development, with ionization collisions in mind.

2. Publications

(a) The manuscript appearing as appendix B of the previous status report No. 5, Oct. 8, 1974 - Jan. 8, 1975 and entitled,

"A Ten-Channel Eikonal Treatment of Differential and
Integral Cross Sections and of the (λ, χ) Parameters
for the $n = 2$ and 3 Excitations of Helium by Electron-
Impact"

by M. R. Flannery and K. J. McCann has been accepted for publication in J. Phys. B: Atom. Molec. Phys. (1975). The abstract appears on page 3 .

(b) The paper "Excitation in Electron-Metastable Helium Collisions," by M. R. Flannery, W. F. Morrison and B. L. Richmond has now been published in the March 1975 issue of J. Appl. Phys. 46, 1186 (1975). Reprints will be sent when available.

3. Papers Submitted in IX International Conference on the Physics of Electron and Atomic Physics (IX ICPEAC) Seattle, Washington, July 1975.

The following two papers entitled

(a) The λ and χ Angular Correlation Parameters for the 2^1P and 3^1P
Excitations of Helium by Electron-Impact,

(b) A Theoretical Treatment of Direct Atomic Collisions at Intermediate
Energies,

have been submitted. Abstracts appear as Appendix B of this report.

A Ten-Channel Eikonal Treatment of Differential and
Integral Cross Sections and of the (λ, χ) Parameters for the
 $n=2$ and 3 Excitations of Helium by Electron-Impact

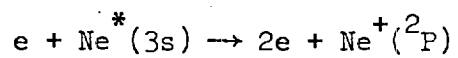
M. R. Flannery and K. J. McCann
School of Physics
Georgia Institute of Technology
Atlanta, Georgia 30332

Abstract. A ten-channel eikonal treatment of the $n=2$ and 3 collisional excitations of helium by incident electrons with energy $E(\text{eV})$ in the range $40 \leq E \leq 500$ is performed. Differential and integral inelastic cross sections are obtained, together with theoretical predictions of the (λ, χ) parameters which provide, as functions of scattering angle θ and E , the orientation and alignment vectors and the circular polarization fraction of the radiation emitted from the n^1P levels. The results are in satisfactory agreement with recent measurements.

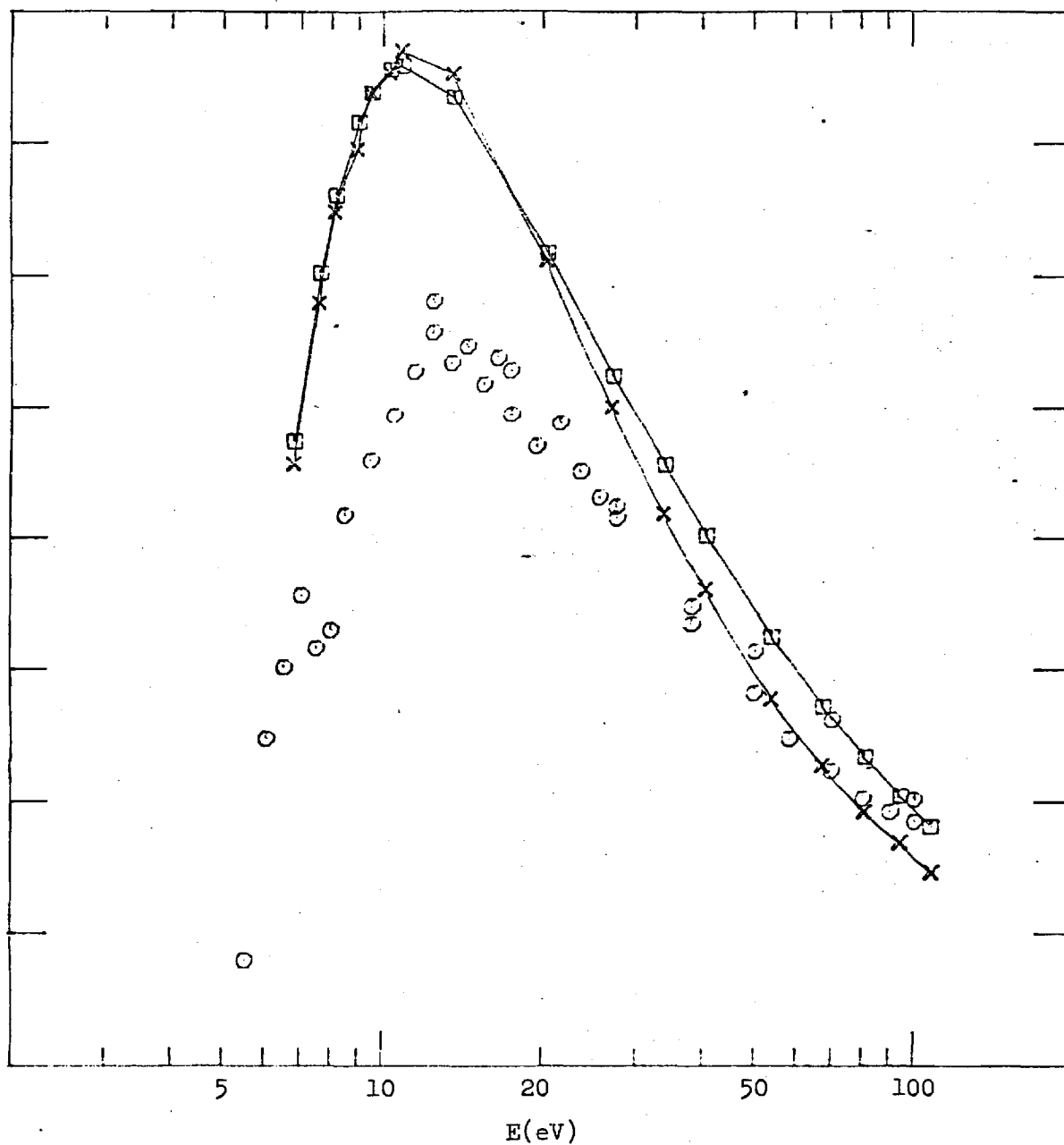
Short Title: $e - \text{He}(1^1S)$ Inelastic Collisions

Physics Abstracts Classification no.: 5.2.8.2

Total Ionization Cross Sections $\sigma(10^{-16} \text{ cm}^2)$ for process,



at Electron-Impact Energy $E(\text{eV})$



X : Born Approximation

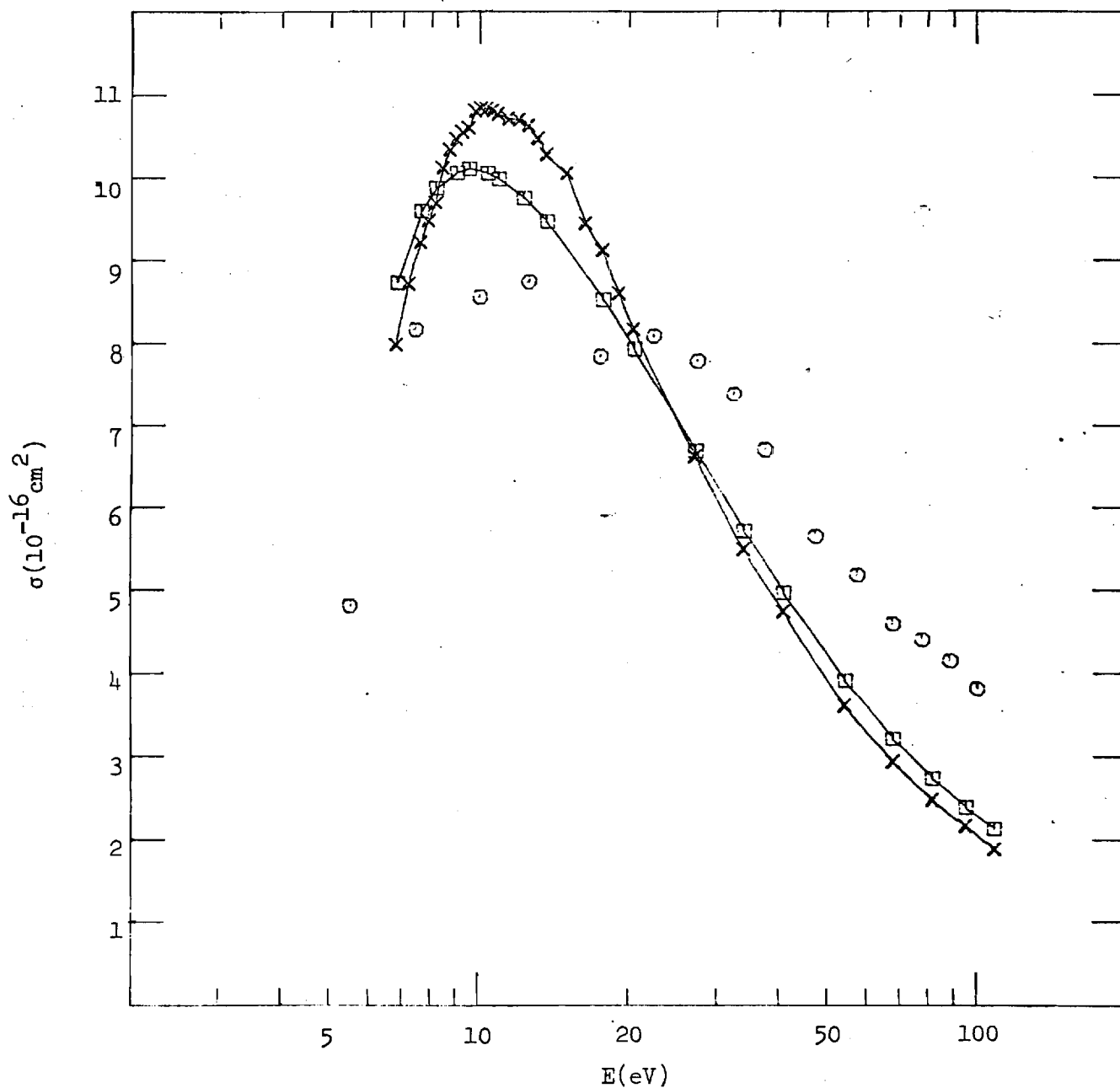
□ : Binary-Encounter Method

⊙ : Measurements of Dixon, Harrison and Smith
(private communication)

Total Ionization Cross Sections $\sigma(10^{-16} \text{ cm}^2)$ for the process,



at Electron-Impact Energy $E(\text{eV})$



X : Born Approximation

□ : Binary-Encounter Method

○ : Measurements of Dixon, Harrison and Smith
(private communication)

Appendix A

"A Theoretical Treatment of Direct Atomic Collisions at Intermediate Energies"

A Theoretical Treatment of
Direct Atomic Collisions at Intermediate Energies

M. R. FLANNERY
School of Physics
Georgia Institute of Technology
Atlanta, Georgia 30332

ABSTRACT

A theoretical description of direct transitions in electron-atom and heavy-particle collisions (without rearrangement) at intermediate energies is developed. The associated T-matrices involve the solution of an integral equation describing elastic scattering by fixed centers. The solution, once determined, can be used to examine the full array of transitions for any given system. An effectively exact description of $e, H^+ - H(n)$ collisions is proposed. With certain simplifying assumptions the multiple scattering problem by fixed centers is solved, thereby providing a useful description of $A - H(n)$ collisions. Various approximate schemes capable of systematic improvement are constructed. The approach can also be applied to direct ionization.

Short Title: Direct Atomic Collisions

Physics Abstracts Classification No.: 5.2.8

1. INTRODUCTION

The theoretical description of atomic collisions at intermediate energies (i.e. beyond the ionization thresholds) is difficult. For low-energy collisions, when a few exit channels are open, the usual close-coupling expansion is, in principle, sound. However, the use of only a limited basis even with a pseudo-state modification prevents proper account of electronic excitation at intermediate energies and cannot naturally be applied to ionization, an instance for which schemes still need to be constructed that are capable of systematic improvement. The Born approximation, which has been applied extensively to high-energy collisions, is clearly inadequate for the intermediate energy region.

In an effort to bridge the energy-gap, various approximate schemes have been proposed, mainly with electron-atom collisions in mind, e.g. distorted-wave approximations, second-order potential methods, multichannel eikonal treatments, eikonal Born series, many-body Green's function techniques, and have all met with varying degrees of success (cf. reviews of Bransden (1973) and of McDowell (1975)).

Nevertheless, most of these methods while performing in practice what the fully quantal close-coupling method formally suggests, are still based on a close-coupling concept which has inherent defects and obvious disadvantages when applied to collisions at intermediate energies. Experiment is achieving a fine precision for electron-atom collisions, i.e. the integral cross sections of e.g. Williams (1974) and of Donaldson et al. (1972), differential cross sections of e.g. Trajmar (1973) and in particular the measurements of Eminyan et al. (1974) of orientation and alignment parameters which are more basic to the collision, all provide independent assessment of the various theoretical models which still exhibit certain inadequacies (Bransden and Winters 1975, McDowell et al. 1975, Flannery and McCann 1975).

In this paper a theoretical method designed particularly for direct collisions at intermediate energies, with no obvious relationship to close-coupling prescriptions, is presented. As will be seen, the approach is effectively exact for e-H and atom A-excited-atom B(n) collisions, and is capable of application and systematic approximation for other collisions. It can also be applied to ionization problems. In the following sections, the theory is developed via operator formalism of (direct) scattering, thereby allowing greater transparency to the inclusion of various important effects and permitting the construction of the resulting equations in a form suitable for subsequent approximation.

2. THEORY: THE BASIC EQUATIONS

The Lippmann-Schwinger operator equation describing the outgoing scattering of two atomic collisions partners by their mutual interaction V is, in terms of the Green's resolvent G and Transition operator T for the collision, given by

$$\psi_i^+ = \phi_i + G_0^+ V \psi_i^+ = \phi_i + G_0^+ V \phi_i = \phi_i + G_0^+ T \phi_i \quad (1)$$

in the center-of-mass system.

The basis set for the unperturbed A-B system with Hamiltonian \mathcal{H}_0 at infinite separation R , and associated Green's resolvent G_0^+ , is, for a fixed arrangement (r, R) ,

$$\phi_i(r, R) = \psi_i(r) \phi_{k_i}(R) \equiv \psi_i(r) \exp i k_i \cdot R \quad (2)$$

a product of the eigenfunctions $\psi_i(r)$ of the internal Hamiltonian H_0 with eigenvalues ϵ_i for the motion of the internal electrons denoted collectively by r with respect to each parent nucleus, and $\phi_k(R)$, eigenstates of the free Hamiltonian K_0 with eigenenergies $\hbar^2 k^2 / 2\mu$ for the undistorted relative motion of A and B with wavevector k and reduced mass μ . Thus, ϕ_i are eigenfunctions in the (direct) channel of $\mathcal{H}_0 = H_0(r) + K_0(R)$ with eigenenergy,

$$E_i = \frac{\hbar^2 k_i^2}{2\mu} + \epsilon_i = \frac{\hbar^2 k_n^2}{2\mu} + \epsilon_n \quad (3)$$

which is conserved throughout the collision. The spatial representation of the scattering function is,

$$\psi_i^+(r, R) = \psi_i(r) e^{i k_i \cdot R} + \iint d\tilde{r}' d\tilde{R}' G_0^+(\tilde{r}, \tilde{R}; \tilde{r}', \tilde{R}') V(\tilde{r}', \tilde{R}') \psi_i^+(\tilde{r}', \tilde{R}') \quad (4)$$

where the Green's function G_0^+ satisfies

$$(E_i - \mathcal{H}_0 + i\epsilon) G_0^+(r, R; r', R') = \delta(r - r') \delta(R - R') \quad (5)$$

and, since the rearrangement (but not dissociative in r) channel is excluded, is therefore given by,

$$G_0^+(r, R; r', R') = \lim_{\epsilon \rightarrow 0^+} \frac{1}{(2\pi)^3} \frac{2\mu}{\hbar^2} \sum_n \psi_n^*(r) \psi_n(r') \int \frac{e^{i\mathbf{k} \cdot (\mathbf{R} - \mathbf{R}')} d\mathbf{k}}{(k_n^2 - k^2 + i\epsilon)} \quad (6)$$

For sufficiently energetic collisions when all excitations (n, k) are open i.e. $k_n^2 > 0$, (6) reduces to (cf. Bransden 1970)

$$G_0^+(r, R; r', R') = - \frac{1}{4\pi} \frac{2\mu}{\hbar^2} \sum_n \frac{\exp i k_n |\mathbf{R} - \mathbf{R}'|}{|\mathbf{R} - \mathbf{R}'|} \psi_n^*(r) \psi_n(r') \quad (7)$$

By considering the asymptotic ($R \rightarrow \infty$) behaviour of (7) in (4), the transition matrix T and associated scattering amplitude f_{if} can be defined with elements,

$$T_{fi} = \langle \phi_f | T | \phi_i \rangle = \langle \psi_f(r) e^{i\mathbf{k}_f \cdot \mathbf{R}} | V(r, R) | \psi_i^+(r, R) \rangle = - \frac{4\pi\hbar^2}{2\mu} f_{if}(\hat{k}_i, \hat{k}_f) \quad (8)$$

Since, in general, exact solutions to (4) for use in (8) do not exist, various methods for constructing the T matrix (or ψ_i^+ and G^+) as a perturbation expansion in the interaction V (assumed weak) give rise to close coupling schemes, exact in principle but limited in practice to a restricted basis set. Moreover, the concept of close-coupling methods is alien to ionization, an instance for which schemes need to be designed which are capable of systematic improvement. There is however another alternative that involves the approximation of G_0^+ in (7) with respect to k_n , rather than G^+ in (1) with respect to V . In heavy particle collisions and in electron-(excited) atom collisions at intermediate and high impact-energies, for example, it is a good approximation to write $k_n \approx k_i$ in (7) which reduces, with the aid of the closure formula for the complete set of internal states n , including the continuum of H_0 ,

$$\sum_n \psi_n^*(r) \psi_n(r') = \delta(r - r') \quad (9)$$

to

$$G_0^+(r, R; r', R') = - \frac{1}{4\pi} \frac{2\mu}{\hbar^2} \frac{\exp i k_i |\mathbf{R} - \mathbf{R}'|}{|\mathbf{R} - \mathbf{R}'|} \delta(r - r') \quad (10)$$

replaces the many-particle Green's function in effect by the free-particle Green's function, with the result, the total scattering function is,

$$\psi_i^+(\underline{r}, \underline{R}) = \psi_i(\underline{r}) e^{i\vec{k}_i \cdot \underline{R}} - \frac{1}{4\pi} \frac{2m}{\hbar^2} \int \underline{dR'} \frac{e^{i\vec{k}_i \cdot |\underline{R}-\underline{R'}|}}{|\underline{R}-\underline{R'}|} V(\underline{r}, \underline{R'}) \psi_i^+(\underline{r}, \underline{R'}) \quad (11)$$

a form which suggests the following substitution,

$$\psi_i^+(\underline{r}, \underline{R}) = \psi_i(\underline{r}) \chi_i^+(\underline{r}, \underline{R}) \quad (12)$$

where the new function χ_i^+ satisfies the integral equation

$$\chi_i^+(\underline{r}, \underline{R}) = e^{i\vec{k}_i \cdot \underline{R}} - \frac{1}{4\pi} \frac{2\mu}{\hbar^2} \int \underline{dR'} \frac{e^{i\vec{k}_i \cdot |\underline{R}-\underline{R'}|}}{|\underline{R}-\underline{R'}|} V(\underline{r}, \underline{R'}) \chi_i^+(\underline{r}, \underline{R'}) \quad (13)$$

This equation (13) describes the elastic scattering of a fictitious projectile of original wavenumber k_i by a fixed multicentered electrostatic interaction $V(\underline{r}, \underline{R})$. The transition matrix (8) for the A-B collision is therefore,

$$T_{fi} = \langle \psi_f(\underline{r}) e^{i\vec{k}_f \cdot \underline{R}} | V(\underline{r}, \underline{R}) | \psi_i(\underline{r}) \chi_i^+(\underline{r}, \underline{R}) \rangle \quad (14a)$$

which may be alternatively written as

$$T_{fi} = \langle \psi_f(\underline{r}) | T_e(\underline{k}_i, \underline{k}_f; \underline{r}) | \psi_i(\underline{r}) \rangle_{\underline{r}} \quad (14b)$$

where

$$T_e(\underline{k}_i, \underline{k}_f; \underline{r}) = \langle e^{i\vec{k}_f \cdot \underline{R}} | V(\underline{r}, \underline{R}) | \chi_i^+(\underline{r}, \underline{R}) \rangle_{\underline{R}} \quad (15a)$$

the T-matrix for scattering by the fixed structureless potential $V(\underline{r}, \underline{R})$ is determined both on ($k_i = k_f$) and off ($k_i \neq k_f$) the energy shell. Thus (14) emphasizes directly the unique role of elastic scattering in inelastic collisions and involves, as the only unknown (15a) or alternatively the full solution to the equation,

$$\left[-\frac{\hbar^2}{2\mu} \nabla_{\underline{R}}^2 + V(\underline{r}, \underline{R}) \right] \chi_i^+(\underline{r}, \underline{R}) = E_i \chi_i^+(\underline{r}, \underline{R}), \quad E_i = \hbar^2 k_i^2 / 2\mu \quad (15b)$$

subject to the usual outgoing scattering condition. Note that all the information obtained in general by numerical integration of (15) is used in T_{fi} .

The scheme is therefore efficient in that the work entailed in the solution

χ_i^+ to (15b) is not redundant, as opposed to other methods based on perturbation series (e.g. closely-coupled methods) for which a solution is integrated out from the origin in an effort to obtain only its asymptotic behavior. The full knowledge of χ_i^+ for all R is, of course, associated with the fact that the full T-matrix (15a), with elements on and off the energy shell, is required (see Appendix). Moreover, once $\chi_i^+(r, R)$ is obtained for a given scattering system, then it is preset for examination of all transitions within the system, i.e. χ_i^+ needs to be determined only once for a given system. Note that in the limit of zero V , χ_i^+ in (15b) is a plane wave and (14) reproduces the Born approximation.

3. BASIS FOR SYSTEMATIC APPROXIMATION

Thus, the (inelastic) scattering of composite structures is reduced to the solution of elastic scattering by fixed potential centers, in general multiple, positioned at the origin and at r_i and given by

$$V(r, R) = V_0(R) + \sum_{i=1}^N V_i(r_i - R) \quad (16)$$

a series of two-body interactions. Although the following analysis can be immediately generalized so as to cover complex targets, assume for simplicity that the target is a one-electron atom ($N=1$), and that the projectile is structureless. Introduce

$$C_i^\pm = \phi_i + \frac{1}{E_i - K_0 \pm i\epsilon} V_0 C_i^\pm = \phi_i + \frac{1}{E_i - K_0 - V_0 \pm i\epsilon} V_0 \phi_i \quad (17)$$

the solution for elastic scattering by V_0 in (16) alone. With the aid of (17) and of

$$(E_i - K_0 + i\epsilon)^{-1} = (E_i - K_0 - V_0 + i\epsilon)^{-1} [1 - V_0 (E_i - K_0 + i\epsilon)^{-1}] \quad (18)$$

the integral equation

$$\chi_i^+ = \phi_i + \frac{1}{E_i - K_0 + i\epsilon} (V_0 + V_1) \chi_i^+ \quad (19)$$

can be rewritten as,

$$\chi_i^+ = C_i^+ + \frac{1}{E_i - K_0 - V_0 + i\epsilon} V_1 \chi_i^+ \quad (20)$$

which, by further application of (18) with $K_0 \rightarrow K_0 + V_0$ and $V_0 \rightarrow V_1$, $V = V_0 + V_1$ can be alternatively written as

$$\chi_i^+ = C_i^+ + \frac{1}{E_i - K_0 - V + i\epsilon} V_1 C_i^+ \quad (21)$$

Hence, (14) is now exactly,

$$\begin{aligned} T_{fi} &= \langle \psi_f(r) \phi_f(R) | V | \psi_i(r) C_i^+(R) \rangle \\ &+ \langle \psi_f(r) \phi_f(R) | V | \psi_i(r) (E_i - K_0 - V + i\epsilon)^{-1} V_1 C_i^+(R) \rangle \end{aligned} \quad (22)$$

in a form suitable for approximation. For example, when the effect arising from $V_0 \gg$ the effect from V_1 then χ_i^+ in (21) is simply the extra scattering of C_i^+ by V_1 . When this additional scattering can be neglected, $\chi_i^+ = C_i^+$ and

$$T_{fi} \approx T'_{fi} = \langle \psi_f(r) \phi_f(R) | V | \psi_i(r) C_i^+(R) \rangle \quad (23)$$

a formula identical with the Coulomb projected-Born result of Geltman (1971) when V_0 is a Coulomb field. Thus this approximation entirely neglects the second term of (22), a procedure valid only for very close encounters with the target nucleus.

Another alternative and exact form of (14) suitable for approximation is obtained with the aid of $\langle \phi_f |$ in (17) and of (20) in (14) to yield

$$T_{fi} = \langle \psi_f \phi_f | V_0 | \psi_i C_i^+ \rangle + \langle \psi_f C_f^- | V_1 | \psi_i \chi_i^+ \rangle \quad (24)$$

a two-potential scattering formula. Inserting (21) in the RHS of (24),

$$\begin{aligned} T_{fi} &= \langle \psi_f \phi_f | V_0 | \psi_i C_i^+ \rangle + \langle \psi_f C_f^- | V_1 | \psi_i C_i^+ \rangle \\ &+ \langle \psi_f C_f^- | V_1 | \psi_i (E_i - K_0 - V + i\epsilon)^{-1} V_1 C_i^+ \rangle \end{aligned} \quad (25)$$

such that if V_1 is small then V_1^2 can be neglected with the result

$$T_{fi} \approx T_{fi}^{\sim} = \langle \psi_f \phi_f | V_0 | \psi_i c_i^+ \rangle + \langle \psi_f c_f^- | V_1 | \psi_i c_i^+ \rangle \quad (26)$$

which is the distorted Born-wave formula used for elastic scattering by $V(\underline{r}, R)$ in an inelastic matrix element (14). The approximation T_{if}^{\sim} is obviously much more sophisticated than the customary DWBA to close coupling formulae for which the distorted waves refer to distortion by the static interactions $\langle \psi_n | V | \psi_n \rangle$ of the initial and final channels and not as, in this case, to distortion by the full electrostatic interaction $V_0(R)$.

While only a few schemes suitable for approximation of (14) have been constructed above, there are several instances for which exact or effectively exact solutions can be obtained as follows.

4. SOLUBLE MODELS

(a) Charged Particle-Atom Collisions:

Consider collisions between structureless particles of charge Ze with atomic hydrogen. The function χ_1^+ is therefore the solution for elastic scattering by two fixed centers of charge of opposite sign ($\pm Ze$), in general, or, in particular, by a fixed dipole, when distant encounters R are dominant, or by a Coulomb field when close collisions with the nucleus are important. In the general case (a situation analogous to the exact determination of the continuum orbital of H_2^+ by Bates, Öpik and Poots (1953) and by Flannery and Öpik (1965)), the introduction of the prolate spheroidal coordinates,

$$\begin{aligned} \lambda &= (\underline{R} + |\underline{R} - \underline{r}|)/r, & 1 \leq \lambda \leq \infty \\ \mu &= (\underline{R} - |\underline{R} - \underline{r}|)/r, & -1 \leq \mu \leq 1 \end{aligned} \quad (27)$$

and Φ , the angle of rotation of R about the r axis, with the substitution,

$$\chi_1^+(r, R) = \Lambda(\lambda|r) M(\mu|r) e^{im\Phi} \quad (28)$$

permits the separation of the Schrödinger equation (15) into the following two second-order differential equations,

$$\frac{d}{d\lambda} \left[(\lambda^2 - 1) \frac{d\Lambda^{(m)}}{d\lambda} \right] + \left[A + p^2 \lambda^2 - \frac{m^2}{\lambda^2 - 1} \right] \Lambda^{(m)}(\lambda) = 0 \quad (29a)$$

in which $p = \frac{1}{2} (k_1 r)$, and

$$\frac{d}{d\mu} \left[(1 - \mu^2) \frac{dM^{(m)}}{d\mu} \right] + \left[-A - p^2 \mu^2 + 2r Z\mu - \frac{m^2}{1 - \mu^2} \right] M^{(m)}(\mu) = 0 \quad (29b)$$

coupled by a separation constant A . Eq.(29a), which defines the radial Spheroidal function, can be solved exactly as a linear combination of radial Bessel functions (cf. Flammer 1956). Moreover, with the substitution,

$$\Lambda = (1 - \lambda^2)^{-\frac{1}{2}} \Omega(\lambda) \quad (30)$$

then (29a) reduces to

$$\frac{d^2 \Omega}{d\lambda^2} + \left[\frac{p^2 \lambda^2 + A}{\lambda^2 - 1} + \frac{1 - m^2}{(\lambda^2 - 1)^2} \right] \Omega(\lambda) = 0 \quad (31)$$

which is capable of direct numerical solution subject to $\Omega(1) = 0$, and to an appropriate asymptotic form, correctly normalized. To initiate the integration procedure, a series solution for small λ can be constructed to give,

$$\Omega^{(m)}(\lambda) = (\lambda^2 - 1)^{\frac{m+1}{2}} \left[1 - \frac{K(\lambda-1)}{2(m+1)} + \frac{1}{4} \left\{ K - 2p^2 + \frac{K^2}{2m+1} \right\} \frac{(\lambda-1)^2}{m+2} + \dots \right],$$

$$K = A + p^2 + m(m+1) \quad (32)$$

In the limit as $r \rightarrow 0$, (29b) reduces to the equation for the associated Legendre functions $P_n^m(\mu)$ and a series solution to (29b) can be obtained with the form,

$$M^{(m)}(\mu) = \sum_{s=0}^{\infty} d_s^m(p, r) P_{m+s}^m(\mu) \quad (33)$$

where the coefficients d_r^m satisfy certain recursion relations. Hence, the full solution χ_i^+ which contains all the information on distortion, is known, but must first be transformed from the coordinate axis in which \underline{r} is fixed to a space-fixed frame so that the transition matrix,

$$T_{fi} = \langle \psi_f(\underline{r}) e^{i\mathbf{k}_f \cdot \underline{R}} | \frac{Ze^2}{R} - \frac{Ze^2}{|\underline{R}-\underline{r}|} | \phi_i(\underline{r}) T_{\underline{r}}^{-1}(\lambda|\underline{r}) M(\mu|\underline{r}) e^{im\phi} \rangle \quad (34)$$

can be evaluated exactly (although, not too easily), where $T_{\underline{r}}$ denotes the appropriate transformation-operator.

When distant encounters are important to the elastic scattering, e.g. through small angles, then χ_i^+ corresponds to elastic encounters with a fixed dipole with interaction

$$V(\underline{r}, \underline{R}) \sim + \frac{Ze^2}{R^2} \underline{r} \cdot \hat{\underline{R}} \quad (35)$$

a case for which Mittleman and von Holdt (1965) obtained exact solutions in terms of combinations of spherical (radial) Bessel and angular Legendre functions.

Large-angle elastic scattering results from close-encounters with the nucleus with the result that

$$\chi_i^+(\underline{r}, \underline{R}) \approx \psi_c^+(\underline{R}) = \exp(-\frac{1}{2}\pi\alpha) \Gamma(1 - i\alpha) \exp(i\mathbf{k}_i \cdot \underline{R}) {}_1F_1(i\alpha; 1; -i\mathbf{k}_i \cdot \underline{R}) \quad (36)$$

the Coulomb function with $\alpha = Z(e^2\mu/\hbar^2)k_i$, and T_{if} reduces to the Coulomb-projected Born matrix element of Geltman (1971).

(b) Neutral-(Excited) Atom Collisions

For A-B collisions, an effectively exact solution to χ_i^+ , the fictitious wavefunction describing in general, multiple elastic scattering of A by N-fixed targets within B can be achieved under certain conditions to be later determined. The eventual aim is to incorporate within the theoretical solution the asymptotic scattering amplitudes (or on-the-energy-shell T-matrix elements, assumed known) for two-body interactions between the projectile and each particle n of B.

Since the A-B interaction V is, in general, a sum of two-body interactions

$V_n(R, \underline{r}_n)$ then

$$\chi_i^+ = \phi_i + G_0 \left(\sum_{n=1}^N V_n \right) \chi_i^+ = \phi_i + G_0 V \phi_i + G_0 V G_0 V \phi_i + \dots, \quad (37)$$

where $G_0 \equiv (E - K_0 + i\epsilon)^{-1}$, a one particle Green's operator for free motion of energy E , propagates the effect of each interaction V_n . This equation can be solved by "recycling", as indicated on the RHS, in powers of V , a procedure, while generating the customary Born series, is nonetheless lacking in a simple physical interpretation needed for further approximation in the present instance. The Born series above can however be rearranged so that all terms which involve the scattering of A by each target n of B are combined together, thereby permitting the natural separation of two-body from individual higher-order multiple scattering effects. Each term $(j+1)$ of the Born series is

$$V_n (G_0 V_n) (G_0 V_n) \dots \equiv V_n \left(\frac{1}{E - K_0} V_n \right)^j \quad (38)$$

and hence by following Watson (1953) or Goldberger and Watson (1964) the exact solution can be written as,

$$\chi_i^+ = \phi_i + \frac{1}{E - K_0 + i\epsilon} \sum_{n=1}^N t_n \chi_n \quad (39)$$

a superposition of wavelets χ_n emitted by each target n and given as the solution of

$$\chi_n = \phi_i + \frac{1}{E - K_0 + i\epsilon} \sum_{\substack{n=1 \\ m \neq n}}^N t_m \chi_m \quad (40)$$

a set of coupled integral equations in which the two body transition operators

$$t_n = V_n + V_n \frac{1}{E - K_0 + i\epsilon} t_n \quad (41)$$

correspond, in this case of fixed potentials, to scattering by an isolated

target particle n free from interaction with other particles m . All details of the binding in the $A-B$ collision have already been acknowledged by (14).

Thus, χ_i^+ is the unperturbed function ϕ_i together with wavelets which can be generated by "recycling" (40) to yield

$$\begin{aligned}\chi_n &= \phi_i + G_o \sum_{m \neq n} t_m [\phi_i + G_o \sum_{r \neq m} t_r \{\phi_i + G_o \sum_{s \neq r} t_r (\phi_i + \dots) \dots\} \dots] \\ &= \phi_i + G_o \sum_{m \neq n} t_m \phi_i + G_o \sum_{m \neq n} t_m G_o \sum_{r \neq m} t_r \phi_i + G_o \sum_{m \neq n} t_m G_o \sum_{r \neq m} t_r G_o \sum_{s \neq r} t_s \phi_i\end{aligned}\quad (42)$$

which represents a truly sequential multiple scattering series in which each term corresponds to the arrival mode of the incident particle i on m , e.g. the first term in t_m refers to direct arrival while the second term corresponds to the arrival at m of a wave once scattered previously elsewhere, etc. In contrast the terms $\sum_n V_n G_o \sum_n V_n \phi_i$ in the Born series above include to all orders the important successive interactions with the same particle. Thus (39) - (41) render the key quantity χ_i^+ in a form suitable for approximation to be used in (14).

The only assumption so far is $k_n \approx k_i$ in the many-body Green's function (7), for the direct channel, which entails, from (3),

$$k_i - k_n = \frac{2\mu}{\hbar^2} \frac{(\epsilon_n - \epsilon_i)}{(k_i + k_n)} \approx 0 \quad (43)$$

such that the averaged initial and final relative energy be much less than the internal energy level spacing, a weak-binding approximation only to that part of (7) which describes the relative motion. This assumption causes the introduction of an artificial χ_i^+ , for elastic scattering by fixed multi-center charges. Conversely, the scattering centers have no mechanism for recoil, can be regarded as infinitely heavy and hence binding between the charges will have no effect on the scattering (cf (29)). Thus, the free particle transition operators t_n which emerge in (41) are properties only of the individual scatter n (and projectile).

Additional Approximations. (1) The impact-energy must be uniquely defined between scattering events so that the mean free path λ_M must be much greater than the de Broglie wavelength λ_i of relative motion and hence,

$$\lambda_M \approx (\rho \pi f_n^2)^{-1} \gg \lambda_i = k_i^{-1} \quad (44)$$

where ρ is the number density $N/\frac{4}{3}\pi R^3$ of N particles within the "volume" of B assumed spherical with radius R , and f_n is an effective range for $A-n$ collisions.

(2) The aim is to use elastic scattering data on $A-n$ collisions, i.e. knowledge of only the "on-the-energy-shell" matrix elements of t_n is assumed. The momentum representation of (39) is

$$\chi_i^+ = \phi(k_i) + \frac{1}{(2\pi)^3} \frac{2}{\hbar^2} \sum_{n=1}^N \int \frac{\langle k_\alpha | t_n | k_i \rangle \chi_n(k_\alpha) dk_\alpha}{(k_i^2 - k_\alpha^2 + i\epsilon)} \quad (45)$$

where m is the reduced mass of the $A-n$ system.

As is shown in the appendix, the contribution $\chi_{i(0)}^+$ to (45) arising from "on-the-energy-shell" T matrices with $k_\alpha = k_i$ is

$$\chi_{i(0)}^+(r, R) = \chi_i^+(r, R) \quad R > R_{on}, \quad r \text{ fixed} \quad (46)$$

where R_{on} is a range beyond which V_n vanishes. Thus the use of the associated scattering amplitudes

$$f_n(k_\alpha, k_i) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} \langle k_\alpha | t_n | k_i \rangle, \quad k_\alpha = k_i \quad (47)$$

in (45) entails the condition,

$$f_n \leq r_{nm} \quad (48)$$

where r_{nm} is the (n, m) interparticle spacing within B . Hence,

$$\lambda_M \approx \frac{\max(r_{nm}^3)}{N f_n^2} \geq \frac{f_n}{N} \quad (49)$$

For $H(1s) - H(n)$ collisions at speed v , $f_n \sim 1 \text{ a.u.} \leq n^2$, and $\lambda_M \approx n^2 \text{ a.u.}$
 $\gg 10^{-3}/v$ and thus (44) and (48) are valid for $v \gg 10^{-3}/n^2 \text{ a.u.}$, an easy accomplishment even for $n=1$. Although, electron-atom collisions can be formally excluded because of their long Coulombic ranges, the conditions (44) and (48) are not too restrictive to an approximate treatment.

Therefore, in the spatial representation of (39),

$$\chi_i^+ \approx \chi_{i(0)}^+ = e^{ik_i \cdot R} + \sum_{n=1}^N \int d\tilde{R}' d\tilde{R}'' G_0(\tilde{R}', \tilde{R}'') t_n(\tilde{R}', \tilde{R}'') \chi_n(\tilde{R}'') \quad (50)$$

with

$$t_n(\tilde{R}', \tilde{R}'') \equiv \langle \tilde{R}' | t_n | \tilde{R}'' \rangle = \frac{1}{(2\pi)^6} \int \langle \tilde{R}' | k' \rangle d\tilde{k}' \langle k' | t_n | k'' \rangle d\tilde{k}'' \langle k'' | \tilde{R}'' \rangle \quad (51)$$

where $\phi_i(\tilde{R}) \equiv \langle \tilde{R} | k_i \rangle = \exp(ik_i \cdot \tilde{R})$. Hence, for a short-range interaction V_n located as a delta function about position r_n of particle n , (51) reduces to

$$t_n(\tilde{R}', \tilde{R}'') = -4\pi \frac{\hbar^2}{2m} f_n \delta(\tilde{R}' - r_n) \delta(\tilde{R}'' - r_n) \quad (52)$$

where f_n is the scattering amplitude associated with the short-range interaction V_n . Therefore with the aid of explicit G_0 and (52),

$$\chi_i^+ = e^{ik_i \cdot R} + \sum_{n=1}^N \frac{\exp ik_i \cdot |R - r_n|}{|R - r_n|} f_n \chi_n(r_n) \quad (53)$$

where, by a similar argument with (40),

$$\chi_n(r_n) = e^{ik_i \cdot r_n} + \sum_{\substack{m=1 \\ m \neq n}}^N \frac{\exp ik_i \cdot |r_n - r_m|}{|r_n - r_m|} \chi_m(r_m), \quad n=1, 2, \dots, N \quad (54)$$

a set of N -algebraic (rather than integral) equations for the numbers $\chi_n(r_n)$.

For $N=2$, the equations can be solved exactly to give

$$\chi_1(r_1) = e^{ik_i \cdot r_1} \left[\left\{ 1 + f_2 \left(\frac{e^{ik_i \cdot r_{12}}}{r_{12}} \right) e^{-ik_i \cdot r_{12}} \right\} / \left(1 - \frac{f_1 f_2}{r_{12}^2} e^{2ik_i \cdot r_{12}} \right) \right] \quad (55)$$

and a similar expression for χ_2 with $\underline{r}_1 \leftrightarrow \underline{r}_2$, to yield an explicit result for $\chi_1^+(\underline{r}_1, \underline{r}_2, \underline{R})$ to be used in (14).

The first term of (55) is the undistorted wavelet emerging from \underline{r}_1 , the second term arises from the reception at 1 of the wavelet emitted by 2, and the denominator of (55) represents the shuttling back and forth. The expansion of (55) for small $r_{1,2} \ll r_{12}$ yield the customary multiple scattering sequence.

Hence, with the knowledge of e-A elastic scattering data, and with (53), and (54) in (14), the general A-H(n) elastic and excitation collisions for all n can effectively be solved exactly subject to the (certain) validity of (43), (44) and (48). Foldy (1945) and Brueckner (1953) originally applied (55) to the scattering of sound waves by two fixed centers, and to the scattering of pi-mesons by deuterons, respectively. The present treatment (37) - (54) has presented the generalized form for χ_i^+ with atomic collisions in mind, and stresses the overall validity for subsequent use in (14) pertinent to A-B collisions.

5. SIMPLE APPROXIMATIONS

As previously noted, the Born approximation and the Coulomb projected-Born approximation (for charged particles) to the transition matrix T_{if} in (14) are reproduced when the elastic scattering function χ_i^+ of (15) is associated either with no interaction V or else with a strong interaction V_0 only with the nucleus, respectively. For V weak, however, a perturbation treatment of (15) yields,

$$\chi_1^+(\underline{r}, \underline{R}) = \phi_1(\underline{R}) + \frac{2\mu}{(2\pi)^3 \hbar^2} \int \frac{\langle \phi_{\underline{k}_\alpha}(\underline{R}') | V(\underline{r}, \underline{R}') | \phi_{\underline{k}_i}(\underline{R}') \rangle}{(k_1^2 - k_\alpha^2 + i\epsilon)} \phi_\alpha(\underline{k}_\alpha) d\underline{k}_\alpha + \dots \quad (56)$$

which, for the charged particle-atom interaction,

$$V(\underline{r}, \underline{R}) = V_0 + V_1 = Ze^2 \left[\frac{1}{R} - \sum_{n=1}^N \frac{1}{|\underline{R} - \underline{r}_n|} \right] \quad (57)$$

reduces, with the aid of Bethé's integral to,

$$\chi_i^+(r, R) = e^{ik_i \cdot R} \left[1 - \frac{8\pi Ze^2 \mu}{(2\pi)^3 \hbar^2} \int \frac{\exp(-ik_\alpha \cdot R) \{1 - \sum_{n=1}^N \exp(ik_\alpha \cdot r_n)\} dK_\alpha}{K_\alpha^2 (K_\alpha^2 - 2k_i \cdot K_\alpha)} \right],$$

$$K_\alpha = k_i - k_\alpha \quad (58)$$

to first order, in which the integral can be explicitly evaluated by contour integration. Moreover for charged particle - (highly) excited atom collisions for which $r_n \gg R$, then (57) is approximately

$$V(r, R) \approx Ze \left[\frac{e}{R} + \sum_{n=1}^N \frac{(-e)}{r_n} \right] \quad (59)$$

with the result that,

$$\chi_i^+(r, R) = \psi_c^+(R) \prod_{n=1}^N \psi_c^+(r_n) \quad (60)$$

products of Coulombic functions (36).

Also, for neutral-neutral collisions A-B when multiple scattering effects can be neglected, (53) yields,

$$\chi_i^+(r, R) = e^{ik_i \cdot R} + f_+ \frac{e^{ik_i \cdot R}}{R} + f_- \sum_{n=1}^N \frac{e^{ik_i \cdot |R-r_n|}}{|R-r_n|} e^{ik_i \cdot r_n} \quad (61)$$

where f_\pm are the elastic scattering amplitudes (in the forward direction) for free H^+ -A and e-A collisions respectively. It is very apparent that a variety of other approximations, even semiclassical, to (15) exist for use in (14), approximations essentially based on the analysis presented in §3 and §4.

A different set of approximations may be generated by considering the contribution to T_{fi} in (14b) that arises from only "on-the-energy-shell" matrix elements T_{el} i.e. $k_f = k_i \hat{k}_f \equiv k'_f$ in T_e of (15a). Thus,

$$T_{fi} = \langle \psi_f(r) | T_{el}(k_i, k'_f; r) | \psi_i(r) \rangle, \quad k_i = k'_f \quad (62)$$

in terms of the amplitude for elastic scattering of the projectile by the fixed potential $V(\underline{r}, \underline{R})$, i.e. the asymptotic behavior of χ_1^+ in (15b) is required. The Born approximation to T_{el} for interaction (16) is

$$T_{el}^{(B)} = \int V_0(\underline{R}) e^{i\mathbf{K} \cdot \underline{R}} d\underline{R} + \sum_{n=1}^N e^{i\mathbf{K} \cdot \underline{r}_n} \int V_n(\underline{R}) e^{i\mathbf{K} \cdot \underline{R}} d\underline{R},$$

$$\underline{K} = k_i(\hat{\underline{k}}_i - \hat{\underline{k}}_f) \quad (63)$$

for use in (62). For Coulomb interactions (57), this procedure yields,

$$T_{fi}^{(B)} = \frac{4\pi}{K^2} [\delta_{fi} - F_{fi}(K)] \quad (64)$$

the Born approximation to T_{fi} in terms of the generalized form factor

$$F_{fi}(K) = \langle \psi_f(r_1, r_2, \dots, r_N) | \sum_{n=1}^N \exp(i\mathbf{K} \cdot \underline{r}_n) | \psi_i(r_1, r_2, \dots, r_N) \rangle \quad (65)$$

Also, for rotational transitions by a pure dipole field, (63) in (64) reproduces the Born result. Hence (62) provides a basis for approximation schemes more accurate than the Born.

The cross section for excitation of all states $f \neq i$ is proportional to,

$$T_{\Sigma} \equiv \sum_{f \neq i} |T_{fi}|^2 = \sum' \langle \psi_i(\underline{r}) | T_e^*(k_i, k_f; \underline{r}) | \psi_f(\underline{r}) \rangle$$

$$\langle \psi_f(\underline{r}) | T_e(k_i, k_f; \underline{r}') | \psi_i(\underline{r}') \rangle \quad (66)$$

which reduces, with the aid of closure (9) and of "on-the-energy-shell" matrices T_{el} to

$$T_{\Sigma} = \langle \psi_i(\underline{r}) | |T_{el}(k_i, k_f; \underline{r})|^2 | \psi_i(\underline{r}) \rangle \quad (67)$$

On using (63) for the Coulomb interactions (57), the Born approximation,

$$T_{\Sigma}^{(B)} = \frac{4\pi}{K^2} [1 - |F_{ii}(K)|^2], \quad \underline{K} = k_i(\hat{\underline{k}}_i - \hat{\underline{k}}_f) \quad (68)$$

follows from (67), which therefore can be used as a basis for more refined approximation.

All of these procedures for the evaluation of χ_i^+ within (14) can be applied of course equally well to ionization as to excitation. However, within the assumption $k_n \approx k_i$, the theoretical formulation in §2 is exact for direct excitation, but not for ionization. This shortcoming (present also in all previous descriptions of ionization) arises by noting that the "two-body" Green's function G_0^+ in (6) describes exactly the channel $a + (b, c)_n, \dots a + (b + c)$ which includes states of excitation $(b, c)_n$ and of dissociation $(b + c)$ only for c in the field of b . The ionization states $(a + b + c)$ belong to a true three-body channel which is only approximately described by the above G_0^+ . The dissociative states $a + (b + c)$ do not actually belong to, nor do they bear any simple relation to, the free states of any physical channel (direct, rearrangement and three-body). They do, however, contain certain projections onto these channels. The projection of the dissociative states in ψ_i^+ is apparently lost by use of the closure relation (9) since ψ_i^+ tends to zero as $r \rightarrow \infty$. However, equation (15) for χ_i^+ must be solved for the full (r, R) range such that χ_i^+ and hence ψ_i^+ does contain some information, as in (56), (58) and (60), on the dissociative states.

In spite of this, however, the present formulation when applied to ionization does represent considerable improvement over previous theoretical approaches e.g. the Born and related approximations assumes χ_i^+ given by the first term of (56), a term containing no information on the three-body channel at all, while the close-coupling method assumes for ψ_i^+ a limited basis set which because of practical difficulties contains no states of dissociation of the system. Moreover, the previous development can be easily generalized so as to include rearrangement or reaction channels, as follows.

6. REARRANGEMENT CHANNELS

The Hamiltonian for the collision system is,

$$\mathcal{H} = \mathcal{H}_{od} + V_d = \mathcal{H}_{ox} + V_x \quad (69)$$

where previously defined quantities associated with either direct channels d or rearranged channels x now contain, for identification purposes, an additional index d or x , respectively. The free Hamiltonians and corresponding eigenfunctions and eigenenergies of the collision system in the absence of the interactions V_d and V_x are respectively

$$\begin{aligned} \mathcal{H}_{od} &= H_o(\underline{r}_d) + K_o(\underline{R}) \\ \phi_{id}(\underline{r}_d, \underline{R}) &= \psi_{id}(\underline{r}_d) \exp(i \underline{k}_{id} \cdot \underline{R}); \quad E_i^{(d)} = \epsilon_i^{(d)} + \frac{\hbar^2 k_{id}^2}{2\mu_d} \end{aligned} \quad (70)$$

and

$$\begin{aligned} \mathcal{H}_{ox} &= H_o(\underline{r}_x) + K_o(\underline{s}) \\ \phi_{ix}(\underline{r}_x, \underline{s}) &= \psi_{ix}(\underline{r}_x) \exp(i \underline{k}_{ix} \cdot \underline{s}); \quad E_i^{(x)} = \epsilon_i^{(x)} + \frac{\hbar^2 k_{ix}^2}{2\mu_x} \end{aligned} \quad (71)$$

where \underline{r}_d and \underline{r}_x denote respectively the internal coordinates of the isolated collision partners in the direct channel and in the channel for which the rearrangement $R \leftrightarrow s$ has occurred between the incident projectile at \underline{R} with an atomic electron at \underline{s} . The wavefunction for the total system therefore satisfies simultaneously,

$$\psi_i^+ = \phi_{id} + (E_i^{(d)} - \mathcal{H}_{od} + i\epsilon)^{-1} V_d \psi_i^+ \quad (72)$$

with its built-in boundary condition and

$$(E_i^{(x)} - H_{ox}) \Psi_i^+ = V_x \Psi_i^+ \quad (73)$$

subject to an outgoing spherical wave alone as $s \rightarrow \infty$. The free particle Green's function for the open channels of (73) is

$$G_o^+(r_x, s; r'_x, s') = -\frac{1}{4\pi} \frac{2\mu_x}{\hbar^2} \sum_n \psi_{nx}(r_x) \psi_{nx}(r'_x) \frac{\exp i k_{nx} |s-s'|}{|s-s'|} \quad (74)$$

with the result that the transition matrix $T_{if}^{(x)}$ for rearrangement can be extracted from the asymptotic form of (74) in (73) to yield

$$T_{if}^{(x)} = \langle \psi_{fx}(r_x) e^{ik_f \cdot s} | V_x(r_x, s) | \Psi_i^+ \rangle \quad (75)$$

Since Ψ_i^+ is given by (72) solved so as to provide an incoming plane wave and an outgoing spherical wave at $R \rightarrow \infty$, then the analysis of §2 is applicable with the result that,

$$T_{if}^{(x)} = \langle \psi_{fx}(r_x) e^{ik_f \cdot s} | V_x(r_x, s) | \psi_{id}(r_d) \chi_i^+(r_d, R) \rangle \quad (76)$$

a form analogous to (14a) for direct collisions. It is therefore apparent that the analysis previously developed in §3 - 6 for the solution χ_i^+ is directly applicable to the determination of the T-matrix for rearrangement collisions.

7. SUMMARY AND CONCLUSIONS

A theoretical description of direct transitions in atomic collisions at intermediate energies has been presented. The method involves the basic approximation that $k_n \approx k_i$ in only that part of the Green's function associated with the relative motion. This approach is effectively exact for e and H^+ direct collisions with $H(n)$ at intermediate energies since, in this instance, the basic premise (which represents the point of departure from following close coupling techniques) that the incident energy be large compared to the energy-level spacings in $H(n)$ is well justified for high n in the case of e -impact and for much lower n (~ 2) for H^+ -impact. In these cases, the problem involves the solution of two second-order differential equations, which can be solved by standard techniques. An attractive feature of the method is that the solution, once determined, can be used to examine the full array of transitions in any given system.

The application to $A-B(n)$ collisions involves the solution of a multiple scattering problem, a solution greatly facilitated by the following two additional assumptions that the de Broglie wavelength of relative motion is small compared to the mean free path and that the effective range of interactions between A and the N fixed particles m of B be smaller than, or of comparable magnitude as, the interspacing between the N -particles. The coupled integral equations then reduce to a set of coupled algebraic equations involving as parameters the scattering amplitudes for the $A-m$ isolated collisions. As is easily apparent, the present approach to $A-B(n)$ collisions is much more rigorous than the previous semiquantal descriptions of Flannery (1970, 1973) in that multiple scattering events are included, and in that excitation (and not only ionization) can be described.

Moreover the method provides a useful description of ionization, one which is capable of systematic improvement and which represents considerable improvement of Born's approximation. It certainly would be of interest however to apply this approach to e-He elastic and inelastic collisions at intermediate energies, a case which is currently receiving serious theoretical and experimental attention (cf. McDowell 1975). Since the applications are obviously numerous, it is intended that future studies will include the generalization to rearrangement channels and detailed examination of certain illustrative atomic and molecular collision processes.

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APPENDIX

The implication on using on-the-energy-shell T matrix elements alone.

The wavefunction for potential scattering by a fixed potential $V(\underline{R})$ is, in channel α ,

$$\psi_{\alpha}^{+}(\underline{R}) = \phi_{\alpha}(\underline{R}) + \int G_0^{+}(\underline{R}, \underline{R}') V(\underline{R}') \psi_{\alpha}^{+}(\underline{R}') d\underline{R}' \quad (A1)$$

$$= \phi_{\alpha}(\underline{R}) + \frac{1}{(2\pi)^3} \frac{2\mu}{\hbar^2} \int \frac{T_{\gamma\alpha} \phi_{\gamma}(\underline{R}) d\underline{k}}{k_{\alpha}^2 - k_{\gamma}^2 + i\epsilon} \quad (A2)$$

with customary notation. Include in (A2) only on-the-energy-shell matrix elements $T_{\gamma\alpha}$ with $k_{\gamma} = k_{\alpha} = k$ and expand the plane wave,

$$\phi_{\gamma}^{(*)}(\underline{R}) = \exp(\pm i \underline{k}_{\gamma} \cdot \underline{R}) = \frac{1}{kR} \sum_{\ell=0}^{\infty} (\pm i)^{\ell} (2\ell + 1) F_{\ell}(k_{\gamma} R) P_{\ell}(\hat{\underline{k}}_{\gamma} \cdot \hat{\underline{R}}) \quad (A3)$$

in terms of the Legendre polynomials P_{ℓ} and the Ricatti-Bessel functions F_{ℓ} which are, given by (Newton 1966),

$$F_{\ell}(kR) = (\frac{1}{2}\pi kR)^{\frac{1}{2}} J_{\ell+\frac{1}{2}}(kR) = (kR) j_{\ell}(kR) \xrightarrow{kR \gg 1} \sin(kR - \frac{1}{2}\ell\pi) \quad (A4)$$

where $J_{\ell+\frac{1}{2}}$ and j_{ℓ} are the Bessel and spherical Bessel functions respectively.

By contour integration, the resulting integral in (A2) is

$$\frac{1}{(2\pi)^3} \int \frac{\exp(i \underline{k}_{\gamma} \cdot \underline{R}) \exp(-i \underline{k}_{\alpha} \cdot \underline{R}') d\underline{k}_{\gamma}}{k_{\alpha}^2 - k_{\gamma}^2 + i\epsilon} = - \frac{1}{4\pi k R R'} \sum_{\ell=0}^{\infty} (2\ell + 1) H_{\ell}^{+}(kR) F_{\ell}(kR') P_{\ell}(\hat{\underline{R}} \cdot \hat{\underline{R}}') \quad (A5)$$

where the Ricatti-Hankel function H_{ℓ}^{+} in terms of the Ricatti-Bessel functions F_{ℓ} and G_{ℓ} of the first and second kinds respectively, is (Newton 1966)

$$H_{\ell}^{+}(kR) = G_{\ell}(kR) + i F_{\ell}(kR) = ikR(j_{\ell} + i\eta_{\ell}) \xrightarrow{kR \gg 1} \exp i(kR - \frac{1}{2}\ell\pi) \quad (A6)$$

in which η_{ℓ} is the spherical Neumann function (or spherical Bessel function of the second kind).

The outgoing Green's function G_0^+ in (A1) can be expanded as

$$G_0^+(\underline{R}, \underline{R}') = - \frac{1}{4\pi k R R'} \frac{2\mu}{\hbar^2} \sum_{\ell=0}^{\infty} (2\ell+1) P_{\ell}(\hat{\underline{R}} \cdot \hat{\underline{R}}') \times \begin{cases} F_{\ell}(kR) H_{\ell}^+(kR'), & R < R' \\ H_{\ell}^+(kR) F_{\ell}(kR'), & R > R' \end{cases} \quad (A7)$$

Hence by comparing (A5) in (A2) and (A7) in (A1), it is seen that the contribution to $\psi_{\alpha(0)}^+$ in (A2) that arises from "on-the-energy-shell" T-matrix elements is related to (A1) by

$$\psi_{\alpha(0)}^+(\underline{R}) = \psi_{\alpha}^+(\underline{R}), \quad R > R_0 \quad (A8)$$

where R_0 is some radius beyond which $V(\underline{R}')$ vanishes. Similar arguments can be applied to (45) and hence (46) holds. Conversely, full information on the scattering function within R_0 entails full knowledge of the T-matrix, knowledge which cannot be provided experimentally.

Appendix B

Papers submitted to IX ICPEAC, July 1975

THE λ AND χ ANGULAR CORRELATION PARAMETERS FOR THE 2^1P AND 3^1P
EXCITATIONS OF HELIUM BY ELECTRON-IMPACT*

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Recently, Eminyan et al.¹ performed notable electron-photon coincidence experiments which provided the ratio,

$$\lambda = |f^{(0)}|^2 / [|f^{(0)}|^2 + 2|f^{(1)}|^2] \quad (1)$$

and the difference

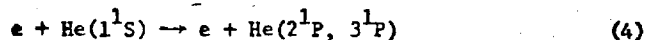
$$\chi = \alpha_1 - \alpha_0 \quad (2)$$

of the phases of the scattering amplitudes

$$f_{if}^{(M)}(E, \theta) = |f_{if}^{(M)}| \exp(i\alpha_M) \quad (3)$$

for the excitation of the n^1P_M substates ($M=0, \pm 1$) of helium by electron-impact as a function of scattering angle θ and impact-energy E .

In this paper, a multichannel eikonal treatment² of the inelastic process,



is performed in which the 1^1S , 2^1S , $2^1P_{0,\pm 1}$, 3^1S , $3^1P_{0,\pm 1}$, and $3^1D_{0,\pm 1,\pm 2}$ states of helium were closely-coupled, hence including the major important couplings between each channel distorted by static interactions, and ensuring conservation of probability. Frozen-core Hartree-Fock wavefunctions were used throughout. In the figure is displayed the resulting λ and χ for the 2^1P and 3^1P excitations as functions of scattering angle θ at incident energy 100 eV, together with the corresponding measured values. Also included, for comparison, are recent theoretical 2^1P -data obtained from the distorted-wave Born approximation (DWBA) of Madison and Shelton³ and from the eikonal DWBA of Joachain and Vanderpoorten⁴, which essentially is a two-state approximation (with back-coupling neglected) to the present more elaborate multichannel treatment.

The figure shows that both eikonal models yield χ -values in closer accord with experiment than does the DWBA which, however, provides better agreement for λ . Also, in spite of the fact that Joachain and Vanderpoorten obtained somewhat improved agreement of χ with experiment when the distorting potentials in the initial and final channels were taken to be the (local) Glauber optical potentials (rather than the customary target static potentials, which yield χ smaller than those shown in the figure) the present refinements to the basic eikonal model has introduced, in general, even closer agreement with experiment.

The figure also shows that the relative agreement between the present

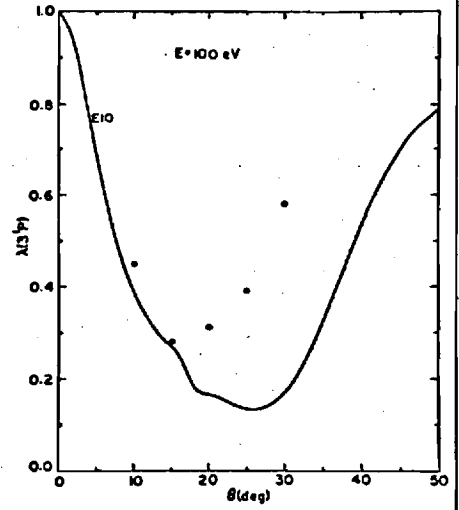
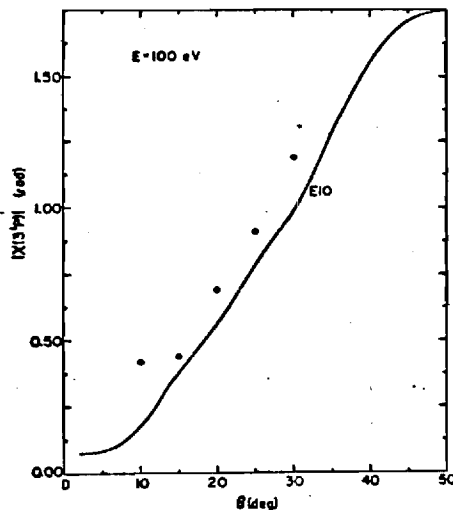
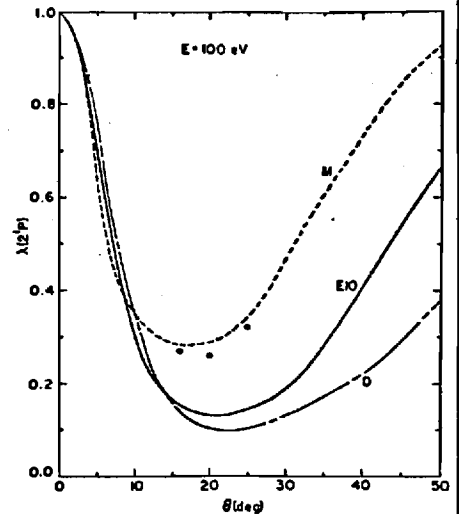
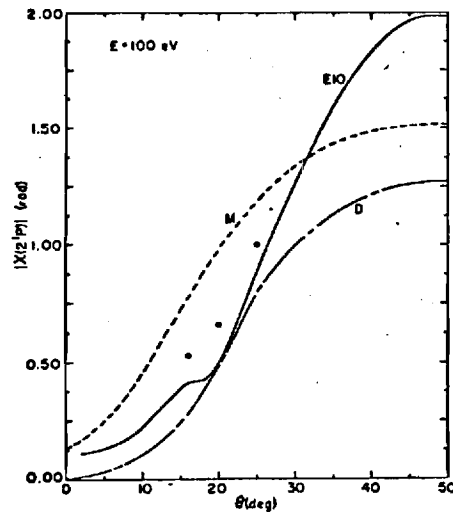


Figure. χ and λ parameters for the n^1P excitation of helium by electrons with energy E (eV). E10: present ten-channel treatment. D: Eikonal distorted-wave Born approximation⁴ (with Glauber optical potential). M: Distorted-wave Born approximation.³ Measurements.¹

approach and measurements becomes improved for the 3^1P excitation, especially at the smaller scattering angles. The apparent structure in $\lambda(3^1P)$ is somewhat reproduced, although shifted to larger scattering angles. There are no other theoretical values available for comparison.

*Research sponsored by the Air Force Aerospace Research Laboratories, Air Force Systems Command, U. S. Air Force Contract No. F33615-74-C04003.

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4. C.J. Joachain and R. Vanderpoorten, J. Phys. B 7, L528 (1974).

A THEORETICAL TREATMENT OF DIRECT ATOMIC COLLISIONS AT INTERMEDIATE ENERGIES*

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For direct transitions in atomic collisions at intermediate and high impact energies, it can be shown that the transition matrix for A-B scattering under their mutual interaction V , reduces to,

$$T_{fi} = \langle \psi_f(\underline{r}) e^{i\mathbf{k}_f \cdot \underline{R}} | V(\underline{r}, \underline{R}) | \psi_i(\underline{r}) \chi_i^+(\underline{r}, \underline{R}) \rangle \quad (1)$$

where χ_i^+ describes the elastic scattering of a fictitious projectile of wave-number k_i by a fixed multicentered interaction $V(\underline{r}, \underline{R})$ and is the solution of

$$\left[-\frac{\hbar^2}{2\mu} \nabla_{\underline{R}}^2 + V(\underline{r}, \underline{R}) \right] \chi_i^+(\underline{r}, \underline{R}) = E_i \chi_i^+(\underline{r}, \underline{R}), \quad E_i = \hbar^2 k_i^2 / 2\mu \quad (2)$$

subject to the usual outgoing condition, where μ is the reduced mass of the A-B system, with internal structure and relative motion at infinite nuclear separation \underline{R} described by $\psi_n(\underline{r})$ and $\exp(i\mathbf{k} \cdot \underline{R})$ respectively. The approach has replaced that part of the many-particle Green's function which describes the relative motion by the free particle Green's function, a procedure which is valid when the energy of the incident projectile is large compared to the internal energy-level spacings of the A-B system.

For charged particle-H(n) collisions, the introduction of prolate spheroidal coordinates (λ, μ, ϕ) and the substitution

$$\chi_i^+(\underline{r}, \underline{R}) = \frac{\Omega(\lambda|\underline{r})}{(1-\lambda^2)^{1/2}} M(\mu|\underline{r}) e^{im\phi} \quad (3)$$

permits the separation of (2) into the following differential equations,

$$\frac{d^2 \Omega}{d\lambda^2} + \left[\frac{p^2 \lambda^2 + A}{\lambda^2 - 1} + \frac{1 - m^2}{(\lambda^2 - 1)^2} \right] \Omega(\lambda) = 0 \quad (4a)$$

in which $p = \frac{1}{2}(k_i r)$, and

$$\frac{d}{d\mu} \left[(1 - \mu^2) \frac{dM^{(m)}}{d\mu} \right] + \left[-A - p^2 \mu^2 + 2\tau Z\mu - \frac{m^2}{1 - \mu^2} \right] M^{(m)}(\mu) = 0 \quad (4b)$$

coupled by a separation constant A . Eq. (4a) is capable of direct numerical solution subject to $\Omega(1) = 0$, and to an appropriate asymptotic form, correctly normalized. A series solution to (4b) can be constructed in terms of associated Legendre polynomials. Thus, on transforming (3) to a fixed frame, (1) can be exactly determined. When distant encounters are important, then χ_i^+ corresponds to small-angle scattering by a fixed dipole, and is therefore known exactly.¹ For close encounters with the nucleus, or large-angle scattering, χ_i^+ is a Coulomb function and (1) reduces to the Coulomb projected Born result.² In the limit of no interaction, χ_i^+ is a plane wave and (1) reproduces the Born result. Other simple approximate schemes³ will be discussed.

The collision A-B(n) involves multiple scattering by N fixed centers. The Born series for (2) can be rearranged so as to separate out the important successive interactions with the same particle, and the coupled integral equations for the one-particle transition operators can be replaced by a set of coupled algebraic equations,³ when (a) the mean free path \gg de Broglie wavelength of relative motion and when (b) the range of the interaction between A and the particles within B is vanishingly small. Thus,³

$$\chi_1^+ = e^{i\mathbf{k}_1 \cdot \mathbf{R}} + \sum_{n=1}^N \frac{\exp i\mathbf{k}_1 \cdot |\mathbf{R} - \mathbf{r}_n|}{|\mathbf{R} - \mathbf{r}_n|} f_n \chi_n(\mathbf{r}_n) \quad (5)$$

where \mathbf{r}_n denotes the position of each scattering center n, and

$$\chi_n(\mathbf{r}_n) = e^{i\mathbf{k}_1 \cdot \mathbf{r}_n} + \sum_{\substack{m=1 \\ m \neq n}}^N \frac{\exp i\mathbf{k}_1 \cdot |\mathbf{r}_n - \mathbf{r}_m|}{|\mathbf{r}_n - \mathbf{r}_m|} \chi_m(\mathbf{r}_m), \quad n=1,2,\dots,N \quad (6)$$

where $f_n \leq r_{nm}$ is the scattering amplitude associated with the short-range A-n interaction. The N-algebraic equations for the numbers $\chi_n(\mathbf{r}_n)$ can be solved by standard techniques. For N=2, the exact solution is immediate, and yields the usual multiple scattering series when $f_{1,2} \ll r_{12}$.

The wavefunction χ_1^+ once determined by the above means or other approximate procedures³ can be used in (1) to study the full array of transitions in any given system. Also, the approach can be applied to ionization, in a form that is capable of systematic improvement.

*Research sponsored by the Air Force Aerospace Research Laboratories, Air Force Systems Command, U.S. Air Force Contract No. F33615-74-C04003.

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2. S. Geltman, J. Phys. B. 4, 1288 (1971).
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GEORGIA INSTITUTE OF TECHNOLOGY

ATLANTA, GEORGIA 30332

July 7, 1975

SCHOOL OF PHYSICS

Air Force Aerospace Research Laboratories

ATTN: ARL/DO

Contract F33615-74-C-4003

Item No. 0002, Sequence No.

Wright-Patterson AFB, OH 45433

SUBJECT: Quarterly R and D Status Report No. 7
Principal Investigator, M. R. Flannery
covering the period 8 April, 75 - 8 July, 75

Gentlemen:

Transmitted herewith are four(4) copies of the subject report.

Should you have any questions or comments regarding this report,
please contact the principal investigator.

Sincerely,

M. R. Flannery.

M. R. Flannery
Professor

MRF:scm

9th
REPORT: ~~Sixth~~ Quarterly R & D Status Report
covering the period 8 April, 1975 - 8 July, 1975

PROJECT-TITLE: Calculation of Electron Impact Cross Sections from
Metastable States in Atomic and Molecular Gases

PRINCIPAL INVESTIGATOR: M. R. Flannery
School of Physics
Georgia Institute of Technology
Atlanta, Georgia 30332

CONTRACT NO: F33615-74-C-4003

SPONSOR CONTACT PERSON: Lt. John F. Prince / Dr. Alan Garscadden
U. S. Air Force
Air Force Systems Command
Bldg. 450, Area B
Hg. 4950th Test Wing, 4950 (PM MA)
Wright-Patterson, AFB, Ohio 45433

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1. Progress acheived during the period 8 April, 1975 - 8 July, 1975

A ten channel eikonal treatment of the $2^{1,3}P$, $3^{1,3}S$, $3^{1,3}P$ and $3^{1,3}D$ excitations of atomic helium, initially in the $2^{1,3}S$ metastable states, by incident electrons with energy $E(\text{eV})$ in the range $5 \leq E \leq 100$ was performed. Integral and differential inelastic cross sections for the processes, $e + \text{He}(2^{1,3}S) \rightarrow e + \text{He}(2^{1,3}P, 3^{1,3}S, 3^{1,3}P, 3^{1,3}D)$ were obtained. Also the angular correlation parameters λ , χ which respectively provided the relative population and relative phase of the collisionally-excited P-magnetic substates, and the circular polarization fraction π of radiation emitted from these P-states were determined as functions of scattering angle θ and E . No measurements exist. The principle of detailed balance was explicitly demonstrated for the $2^1S - 1^1S$ superelastic collision.

2. Publications

(a) The manuscript which appeared as appendix A of the previous status report No. 6, 8 January, 1975 - 8 April, 1975 and entitled "A theoretical treatment of atomic collisions at intermediate energies" by M. R. Flannery has been accepted for publication in J. Phys. B; Atom. Molec. Phys.

(b) The two papers which appeared as Appendix B of the previous status report submitted to the IX ICPEAC, Seattle, Washington, July, 1975, have been accepted and are scheduled for reading on Thursday morning, July 24, 1975 and Wednesday afternoon, July 30, 1975.

3. Results

Integral and differential cross sections for the processes $e + \text{He}(2^{1,3}\text{S}) \rightarrow e + \text{He}(2^{1,3}\text{P}, 3^{1,3}\text{S}, 3^{1,3}\text{P}, 3^{1,3}\text{D})$ were calculated by a ten-channel eikonal treatment of electron-atom collisions. A paper describing this work was written up and was accepted for publication by Phys. Rev. A. It appears as appendix A of this report.

APPENDIX A

A Ten-Channel Eikonal Treatment of Electron-Metastable Helium Collisions:
Differential and Integral Cross Sections for $2^{1,3}\text{P}$ and $n = 3$ Excitations
from $\text{He}(2^{1,3}\text{S})$ and the (λ, χ, π) Parameters

A Ten-Channel Eikonal Treatment of Electron-Metastable Helium Collisions:
Differential and Integral Cross Sections for $2^{1,3}P$ and $n = 3$ Excitations
from $He(2^{1,3}S)$ and the (λ, χ, Π) Parameters *

M. R. Flannery and K. J. McCann
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A ten channel eikonal treatment of the $2^{1,3}P$, $3^{1,3}S$, $3^{1,3}P$ and $3^{1,3}D$ excitations of atomic helium, initially in the $2^{1,3}S$ metastable states, by incident electrons with energy $E(eV)$ in the range $5 \leq E \leq 100$ is performed. Integral and differential inelastic cross sections are obtained. Also the angular correlation parameters λ , χ which respectively provide the relative population and relative phase of the collisionally-excited P-magnetic substates, and the circular polarization fraction Π of radiation emitted from these P-states are determined as functions of scattering angle θ and E . No measurements exist. The principle of detailed balance is explicitly demonstrated for the $2^1S - 1^1S$ superelastic collision.

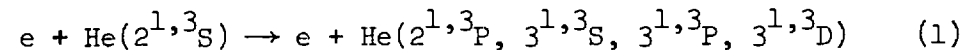
Short Title: $e - He(2^{1,3}S)$ Inelastic Collisions

Analytic Subject Index: 13.4 and 14

I. INTRODUCTION

In contrast to collisions involving ground state atoms, relatively little is known with any great certainty about excitation processes involving atoms initially in a prepared excited state. Such knowledge is very important to the detailed analysis of gaseous-discharges, astrophysical plasmas and formation of excimers¹ (excited metastable molecules, often rare gases).

In this paper, the multichannel eikonal model² which provided a satisfactory account of integral and differential cross sections in e-H(1s) and e-He(1s²) inelastic collisions^{3,4} is applied to the excitation processes,



Frozen-core Hartree-Fock wavefunctions⁵ for helium are used throughout and the $n=(1), 2, \& 3$ channels of each singlet and triplet series will be closely coupled. In addition to the evaluation of integral and differential cross sections for (1), the angular correlation parameters λ and χ , which are more basic to the collision process, and which provide valuable information on the circular polarization of the emitted radiation from the $n^{1,3}\text{P}$ states, will also be studied as a function of impact energy E and scattering angle θ (in the CM-frame).

Contrary to that experienced for transitions from ground atomic states, the Born and Vainshtein, Presnyakov and Sobel'man (VPS) approximations predict¹ that collisional excitations from the $2^{1,3}\text{S}$ metastable-helium state to the $3^{1,3}\text{D}$ and $3^{1,3}\text{S}$ (optically-forbidden) states are more probable than

excitations to the (optically-allowed) $3^{1,3}P$ and $4^{1,3}P$ levels except at incident energies above 100 eV. Hence, couplings between all the states in the $n = 2$ and 3 channels are extremely important and require inclusion for a proper treatment of (1).

II. THEORY

Basic Approximation: In an effort to clarify more fully the basis of the present approach, an alternative derivation of the multichannel eikonal treatment is instructive. The wavefunction for the scattering of two (structured) atoms A and B in general, by their mutual interaction $V(\underline{r}, \underline{R})$ at nuclear separation $\underline{R}(X, Y, Z)$, is

$$\Psi_i^+(\underline{r}, \underline{R}) = \psi_i(\underline{r}) e^{i\mathbf{k}_i \cdot \underline{R}} + \iint d\underline{r}' d\underline{R}' G_O^+(\underline{r}, \underline{R}; \underline{r}', \underline{R}') V(\underline{r}', \underline{R}') \Psi_i^+(\underline{r}', \underline{R}') \quad (2)$$

where the two-particle Green's function G_O^+ , appropriate to \mathcal{H}_O , the Hamiltonian of the unperturbed system of energy E_i at infinite \underline{R} , satisfies

$$(E_i - \mathcal{H}_O + i\epsilon) G_O^+(\underline{r}, \underline{R}; \underline{r}', \underline{R}') = \delta(\underline{r} - \underline{r}') \delta(\underline{R} - \underline{R}') \quad (3)$$

in which the composite internal coordinates are denoted by \underline{r} relative to each parent nucleus. The free particle Green's function, which propagates the effect of the interaction V at $(\underline{r}', \underline{R}')$ to $(\underline{r}, \underline{R})$, can be expanded, in terms of the complete set of eigenfunctions of \mathcal{H}_O , as

$$G_O^+(\underline{r}, \underline{R}; \underline{r}', \underline{R}') = \lim_{\epsilon \rightarrow 0^+} \frac{1}{(2\pi)^3} \frac{2\mu}{\hbar^2} \sum_n \psi_n(\underline{r}) \psi_n^*(\underline{r}') \int \frac{e^{i\mathbf{k} \cdot (\underline{R} - \underline{R}')} d\mathbf{k}}{(k_n^2 - k^2 + i\epsilon)} \quad (4a)$$

where $\psi_n(\underline{r})$ describes the internal structure at infinite nuclear separation R , where the relative motion is planar with propagation vector $\underline{k}(k_x, k_y, k_z)$. For heavy-particle collisions, and for electron-atom inelastic collisions at intermediate and high impact energy, scattering about the forward direction contributes most to the total cross section²⁻⁴, and it is therefore a good approximation to assume that the major contributions to the propagator (4a) arises only from those waves at $Z' < Z$ with $k^2 \approx k_z^2$ such that,

$$G_O^+(\underline{r}, \underline{R}; \underline{r}', \underline{R}') = \lim_{\epsilon \rightarrow 0^+} \frac{1}{(2\pi)^3} \frac{2\mu}{\hbar^2} \int_{-\infty}^{\infty} e^{ik_x(X-X')} dk_x \int_{-\infty}^{\infty} e^{ik_y(Y-Y')} dk_y$$

$$\sum_n \psi_n(\underline{r}) \psi_n^*(\underline{r}') \left[\int_{-\infty}^{\infty} \frac{e^{ik_z(Z-Z')}}{k_n^2 - k_z^2 + i\epsilon} dk_z \right] H(Z - Z') \quad (4b)$$

where $H(Z-Z')$ is the Heaviside step-function (unity for $Z' < Z$ and zero otherwise). Hence, by contour integration, and with introduction of the impact parameter $\rho(X, Y)$,

$$G_O^+(\underline{r}, \underline{R}; \underline{r}', \underline{R}') = \frac{i\mu}{\hbar^2} \sum_s \frac{e^{ik_s(Z-Z')}}{k_s} \delta(\underline{\rho} - \underline{\rho}') H(Z - Z') \psi_s(\underline{r}) \psi_s^*(\underline{r}') \quad (4c)$$

The reduction of (4a) to (4c) can also be obtained by the method of stationary phase (cf. Schiff⁶ and Gerjuoy and Thomas⁷). The multi channel eikonal approximation follows by setting

$$\psi_i^+(\underline{r}, \underline{R}) = \sum_m A_m(\underline{\rho}, Z) \psi_m(\underline{r}) e^{iS_m(\underline{R})} \quad (5)$$

where the eikonal S_m for the relative motion in excitation channel m

under the static interaction

$$V_{nm}(R) = \langle \psi_n(\underline{r}) | V(\underline{r}, R) | \psi_m(\underline{r}) \rangle \quad (6)$$

with $n = m$, satisfies

$$(\nabla_{\underline{S}_m})^2 - i\hbar (\nabla_{\underline{S}_m}^2) = k^2 - \frac{2\mu}{\hbar^2} V_{mm} \equiv K_m^2(R) \quad (7)$$

exactly. The Green's function corresponding to (5) is (4c) with k_s replaced by the local wavenumber K_s , and hence, (2) with (5) reduces to

$$\begin{aligned} \psi_i^+ = \psi_i(\underline{r}) e^{iS_i(R)} - \frac{i\mu}{\hbar^2} \sum_s \int_{R'} \frac{e^{iK_s(Z-Z')}}{K_s} \psi_s(\underline{r}) \delta(\underline{\rho} - \underline{\rho}') H(Z - Z') \\ \sum_{m \neq s} A_m(\underline{\rho}', Z') V_{sm}(R') e^{iS_m(R')} d\underline{\rho}' dZ' \end{aligned} \quad (8)$$

The projection of (8) onto the orthonormal set $\psi_n(\underline{r})$ is

$$\begin{aligned} (A_n e^{iS_n} - \delta_{ni} e^{iS_i}) e^{-iK_n Z} = - \frac{i\mu}{\hbar^2} \int_{-\infty}^Z \frac{e^{-iK_n Z'}}{K_n(\underline{\rho}, Z')} \sum_m A_m(\underline{\rho}, Z') V_{nm}(\underline{\rho}, Z') \\ e^{iS_m(\underline{\rho}, Z')} dZ' \end{aligned} \quad (9)$$

which, on differentiation yields

$$\frac{\partial}{\partial Z} \left[A_n e^{i(S_n - K_n Z)} \right] = - \frac{i\mu}{K_n \hbar^2} \sum_m A_m(\underline{\rho}, Z) V_{nm}(R) e^{i(S_m(R) - K_n Z)} \quad (10)$$

Ignore the second term of L.H.S. of (7) and assume a straight-line trajectory along the Z-axis i.e., $|\nabla_{\underline{S}_n}| \approx \partial S_n / \partial Z \approx K_n$, and $\partial K_n / \partial Z \approx 0$ (equivalent to the neglect of $\nabla_{\underline{S}_n}^2$ in (7)) such that (10) becomes,

$$\frac{i\hbar^2}{\mu} K_n \frac{\partial A_n}{\partial Z} = \sum_{m \neq n} A_m(\underline{\rho}, Z) V_{nm}(R) e^{i(S_m - S_n)} \quad (11)$$

a set of first-order coupled differential equations to be solved for A_n .

Thus, for a finite number of states $n = 1, 2, \dots, N$, the direct transition matrix element T_{fi} or its associated scattering amplitude f_{if} can be evaluated from,

$$T_{fi} = \langle \psi_f(\underline{r}) e^{i\mathbf{k}_f \cdot \underline{R}} | V(\underline{r}, \underline{R}) | \sum_n A_n \psi_n(\underline{r}) e^{iS_n(\underline{R})} \rangle_{\underline{r}, \underline{R}} \equiv -4\pi \frac{\hbar^2}{2\mu} f_{if}(\underline{k}_i, \underline{k}_f) \quad (12a)$$

$$= \sum_n \langle e^{i\mathbf{k}_f \cdot \underline{R}} | V_{fn}(\underline{R}) | A_n(\underline{\rho}, Z) e^{iS_n(\underline{R})} \rangle_{\underline{\rho}, Z} \quad (12b)$$

the basis of the multichannel eikonal treatment.² The transition matrix for rearrangement collisions between the projectile at \underline{R} and a target electron at \underline{r}_i is obtained from (12a) by the $\underline{R} \leftrightarrow \underline{r}_i$ interchange in the wavefunction for the final state f .

The above derivation therefore shows that the multichannel eikonal treatment is based on the following three assumptions: (a) the Green's function (4c), (b) $|VS_n| = \kappa_n$ and (c) a straight-line trajectory, all included within a restricted basis set of N target-states.

Basic Formulae: For a non-degenerate initial state i , the differential cross section for $i \rightarrow f$ excitation is, as a function of scattering angle θ ,

$$\frac{d\sigma}{d\Omega} = \frac{k_f}{k_i} \sum_{M=-L}^L |f_{if}^{(M)}(\theta)|^2 \quad (13)$$

summed over all degenerate magnetic sublevel M of the final level f of the target with angular momentum L , thereby suppressing all knowledge of the populations and phases of each substate. However, two quantities capable of measurement⁸ and calculation as functions of θ and impact energy E , can be defined for excitation of the $n^{1,3}P$ levels, by

$$\lambda = |f_{if}^{(0)}|^2 / [|f_{if}^{(0)}|^2 + 2|f_{if}^{(1)}|^2] \quad (14)$$

and

$$\chi = \alpha_1 - \alpha_0 \quad (15)$$

where α_M is the phase of the scattering amplitude

$$f_{if}^{(M)} = |f_{if}^{(M)}| \exp(i\alpha_M) \quad (16)$$

and where the axis of quantization of the target is taken along the incident Z-direction defined by \hat{k}_i . The parameter λ is the relative contribution arising from the $M = 0$ sublevel to (13) while χ is a measure of the coherence between the excitations of the $M = 0$ and 1 sublevels i.e. phase difference between the corresponding oscillating and rotating dipoles, respectively. A related quantity therefore is the circular polarization fraction of the radiation emitted from the $n^{1,3}P$ levels in a direction perpendicular to the (assumed) XZ-plane of the scattering,

$$\Pi = -2[\lambda(1 - \lambda)]^{1/2} \sin \chi \equiv \overline{\Delta L}_y \quad (17)$$

where $\overline{\Delta L}_y$ is the expectation value of the angular momentum transferred in the Y-direction during the collisions.⁹

The basic formula (12) for the scattering amplitude can be further reduced for two-particle interactions for which $V_{fi}(R) = V_{fi}(\rho, Z) \exp(i\Delta\phi)$, to yield²

$$f_{if}(\theta, \phi) = -i^{\Delta+1} \int_0^\infty J_\Delta(K'\rho) [I_1(\rho, \theta) - i I_2(\rho, \theta)] \rho d\rho \quad (18)$$

where J_Δ are Bessel functions of integral order ($M_i - M_f$) the change in magnetic quantum number, and where K' is the XY-component $k_f \sin \theta$ of the

momentum-change $K = k_i - k_f$. The collisions functions

$$I_1(\rho, \theta; \alpha) = \int_{-\infty}^{\infty} \kappa_f(\rho, Z) \left[\frac{\partial C_f(\rho, Z)}{\partial Z} \right] \exp(i\alpha Z) dZ \quad (19)$$

and

$$I_2(\rho, \theta; \alpha) = \int_{-\infty}^{\infty} \left[\kappa_f(\kappa_f - k_f) + \frac{\mu}{\hbar^2} V_{ff} \right] C_f(\rho, Z) \exp(i\alpha Z) dZ \quad (20)$$

contain a dependence on the scattering angle θ via

$$\alpha = k_f(1 - \cos \theta) = 2k_f \sin^2 \frac{\theta}{2} \quad (21)$$

the difference between the Z-component of the momentum change K and the minimum change $k_i - k_f$ in the collision. The coupling (phase ϕ -independent) amplitudes C_f are solutions of the following set of N-coupled differential equations

$$\begin{aligned} \frac{i\hbar^2}{\mu} \kappa_f(\rho, Z) \frac{\partial C_f(\rho, Z)}{\partial Z} + \left[\frac{\hbar^2}{\mu} \kappa_f(\kappa_f - k_f) + V_{ff}(\rho, Z) \right] C_f(\rho, Z) = \\ \sum_{n=1}^N C_n(\rho, Z) V_{fn}(\rho, Z) \exp i(k_n - k_f) Z, \quad f = 1, 2, \dots, N \end{aligned} \quad (22)$$

solved subject to the asymptotic boundary condition $C_f(\rho, -\infty) = \delta_{if}$.

III. RESULTS AND DISCUSSION

In order to express the interaction matrix elements (6) as analytical functions of R it proves convenient to transform the frozen-core Hartree-Fock wavefunctions of Cohen and McEachran.⁵ Thus, the spatial wavefunctions for the $n = 1 - 3$ states of helium are,

$$\psi_{1s,n\ell m}(r_1, r_2) = N_{n\ell} [\phi_o(r_1) \phi_{n\ell m}(r_2) \pm \phi_o(r_2) \phi_{n\ell m}(r_1)] \quad (23)$$

in which the \pm signs refer to the symmetric (singlet) and antisymmetric (triplet) cases, respectively. The frozen, inner $1s$ -orbital is (in a.u.)

$$\phi_o(r) = 2^{5/2} e^{-2r} Y_{00}(\hat{r}) \quad (24)$$

and the orbital for the second electron in state $(n\ell m)$ is rewritten (in a.u.) as,

$$\phi_{n\ell m}(r) = \sum_{N=\ell+1}^{J-\ell} B_N^{n\ell} e^{-\beta r} r^{N-1} Y_{\ell m}(\hat{r}), \quad \beta = \frac{2}{n} \quad (25)$$

where J is the maximum number of linear coefficients $B_N^{n\ell}$ given in terms of Cohen and McEachran's original parameters $a_j^{n\ell}$ by³

$$B_N^{n\ell} = \sum_{j=N+\ell}^J \frac{(-1)^{N-\ell} 2^\ell (j!)^2 (2\beta)^{N-\ell-1}}{(N-\ell-1)! (j-N-\ell)! (N+\ell)!} a_j^{n\ell}, \quad N = 1, 2, \dots, J \quad (26)$$

The above transformation (26) facilitates subsequent evaluation of the e-He interaction matrix elements

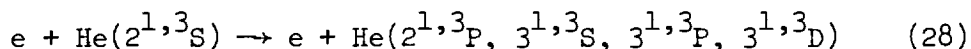
$$V_{ij}(R) = \langle \phi_i(r_1, r_2) | -\frac{2}{R} + \frac{1}{|R-r_1|} + \frac{1}{|R-r_2|} | \phi_j(r_1, r_2) \rangle \quad (27)$$

as analytical functions of R , for all combinations of i and j appropriate to a ten-state treatment. In addition to the $n = 2$ and 3 channels, the superelastic 1^1S -channel was included for singlet-singlet transitions.

The above frozen-core approximation for He implies that correlation effects between the inner and outer atomic electrons have been explicitly neglected (although some implicit account is assumed by virtue of (25)), and is therefore effectively exact for highly-excited Rydberg states. Metastable helium is unique in that its excitation energy, 19.8 eV above the ground state, is the largest of all the singly-excited atoms, its outer electron is relatively weakly bound ~ 4.8 eV, and the mean interelectronic separation in the 2^1S state is $\sim 5.3 a_0$. Therefore, the main response of target helium to the projectile electron is expected to arise from the outer electron such that the use of a frozen-core orbital for the inner electron within a close-coupling scattering wavefunction (5) is expected to be quite accurate. This is further supported by the fact that the dominant contributions to the integral inelastic cross sections for singly-excited transitions arise from small scattering angles $\theta \leq 20^\circ$ (cf. fig. 5) which result from distant encounters. At the lowest impact-energy (5 eV), however, the angular distribution tends to become more isotropic such that close encounters are gaining in relative importance. This situation is difficult to assess without resort, not only to correlated atomic wavefunctions, but also to a more elaborate scattering formalism involving some mechanism which permits response of the inner electron ^{to the projectile.} If correlation effects with the inner electron are to be included in the atomic function, then similar refinements involving its interaction with the projectile must also be included in a more elaborate scattering formalism, not based on an atomic close-coupling expansion valid only for weak perturbations, but on some perturbed three-body expansion. It is worth noting that the atomic wavefunctions adopted in this paper are the most accurate ones used to date in any scattering description more refined than Born's approximation.

8(a) follows (8)

In figures(1) - (3) are displayed the integral cross sections for the processes



at incident electron-energies $E(\text{eV})$ in the range $5 \leq E \leq 100$, together with comparison Born values determined from the highly accurate form factors of Kim and Inokuti.¹⁰ It is worth noting that the coupled-state calculations were much more time-consuming (~ 5 hrs. U1108) than a corresponding treatment of excitation from the ground state^{3,4} which involved ~ 1 hr. U1108. This additional time resulted from the closeness of the initial 2^1S with neighboring 2^1P channels, which because of their long-range static and coupled interactions, necessitated the inclusion of large-impact parameters $\rho \sim 100$ a.u. so as to achieve convergence for both the solutions of the coupled equations (22) and for the integration (18) involving the Bessel functions which oscillated rapidly at these large ρ .

In general, transitions between singlet states of given configurations are much more probable than the corresponding triplet-triplet transitions. Figs. (1-3) show that the multichannel treatment preserves the Born predictions of the relative importance of transitions to the $2^{1,3}\text{P}$, $3^{1,3}\text{D}$, $3^{1,3}\text{S}$ and $3^{1,3}\text{P}$ states, written in order of decreasing probability, except at $E \geq 25$ eV and ≥ 70 eV when excitations of the 3^1P and 3^3P states respectively become greater than the $3^{1,3}$ excitations. The results of Burke et al.,¹¹ who used simple analytic wavefunctions,

Note that the cross sections $\sigma(n\ell m)$ for excitation of the $n^{1,3}P$ ($m = \pm 1$) and $3^{1,3}D(m = \pm 2)$ substates dominate the cross sections $\sigma(n\ell)$ for excitation of the respective levels ($n\ell$) at high impact-energies. This behavior is consistent with the high-energy limit to Born's approximation which predicts that the ratio $\sigma(n\ell m)/\sigma(n\ell)$ is $2|P_{\ell}^m(0)|^2/(2\ell+1)$ where the associated Legendre functions $P_{\ell}^m(0)$ are zero for odd ($\ell-m$), and are largest when $|m| = \ell$. Alternatively, when impulsive conditions prevail, the change ΔL_y in the angular momentum perpendicular to the XZ-scattering-plane is directly proportional to the linear momentum-change $K \approx 2k_i \sin \frac{1}{2}\theta$ which is perpendicular to the incident direction and which vanishes for high-energy scattering in the forward direction, thereby permitting angular momentum changes only in the Z-direction to occur.

closely coupled the $n=1$ and 2 states for total (system) angular momentum $L = 0$ and 1 and used a Born approximation for higher L , are also displayed in Fig. 1, for comparison. A remarkable feature is that the Born limit is approached by the Eikonal treatment at fairly low E , especially for the singlet transitions. Validity of Born's approximation has, as yet, not been fully explored for collisions involving excited atoms, although here the criterion $E \gg (\epsilon_f - \epsilon_i)$, the excitation energy, is satisfied for E much lower than that normally required for excitation from the ground-state. The undulations in the $2^{1,3}S - 3^{1,3}P$ cross sections in Figs. 2-3 are direct consequences of a zero in the corresponding form factors at non-zero momentum-change K . In general, at low E , the stronger (optically-forbidden) transitions are less affected by couplings than the weaker $2^{1,3} - 3^{1,3}P$ transitions which, however, converge more rapidly onto the Born limit at higher E .

The present ten-channel cross sections σ_M for excitation of magnetic sublevel M of (28) are displayed in Table 1. Cross sections for the $2^1S - 1^1S$ superelastic collision are also provided such that the detailed balance relation

$$k_i^2 \sigma_{if}(k_i) = k_f^2 \sigma_{fi}(k_f), \quad k_i^2 = k_f^2 + \frac{2\mu}{\hbar^2} (\epsilon_f - \epsilon_i) \quad (29)$$

between the forward and reverse rates for the process can be tested, thereby permitting assessment of the overall accuracy of the calculations. Thus, the crosses in Figure 4, refer to the present $2^1S - 1^1S$ results for the LHS of (29) with $E \geq 5$ eV, while the dots, representing the RHS of (29), are

taken from a previous ten-channel treatment⁴ of the 2^1S -excitation from the ground state for $E \gtrsim 40$ eV. The maximum deviation corresponds to an error of 2.5% in σ .

The plane-polarization fractions¹²

$$P(n^1P - n^1S) = \frac{\sigma_o - \sigma_1}{\sigma_o + \sigma_1} ; P(n^3P - 2^3S) = \frac{15(\sigma_o - \sigma_1)}{41\sigma_o + 67\sigma_1} \quad (29a)$$

and

$$P(3^1D - 2^1P) = \frac{3(\sigma_o + \sigma_1 - 2\sigma_2)}{5\sigma_o + 9\sigma_1 + 6\sigma_2} ; P(3^3D - n^3P) = \frac{213(\sigma_o + \sigma_1 - 2\sigma_2)}{671\sigma_o + 1271\sigma_1 + 1058\sigma_2} \quad (29b)$$

for the dipole radiation emitted from the excited states are presented in Table 2. The effect of the couplings on the magnetic substates is strongly evident, particularly for the P-S transitions, when little correspondence is exhibited between columns 2 and 4 and between 3 and 5.

Differential Cross Sections: In Fig. 5 are displayed the differential cross sections for the singlet-singlet transitions, as a function of scattering-angle θ and impact-energy $E(\text{eV})$. The structure present in the 3^1P excitation but absent in the 2^1P excitation is a direct consequence of the very important, strong $3^1D(m = 0, \pm 1, \pm 2) - 3^1P$ close-couplings which affect the magnetic substates of 3^1P more than do the $1^1P - 1^1S$ couplings. The relative importance of close-encounters (large-angle scattering) for optically-forbidden versus optically allowed transitions is exhibited by the slower decrease with θ in Fig. 5(b, d) relative to Fig. 5(a, c).

No measurements or other theoretical calculations are available. However, since excitation from the 1^1S state was very-well described

(when compared with experiment) by the multichannel eikonal approach

$0 \leq \theta \leq 40^\circ$, a range contributing effectively all of the integral cross section, the data in Fig. 5 is presumed quite accurate for small-angle scattering. Electron exchange effects, important for large-angle scattering,⁴ have been explicitly neglected, although some (small) allowance does result by virtue of a multistate target expansion. Also differential cross sections for excitation of the m-substates are available from the authors. No measurements, as yet, exist, although, when various theoretical and experimental data for the $1^1S-2^1P_0$ differential magnetic sublevel cross sections were compared for electron-helium scattering at 60 eV and 80 eV, Chutjian and Srivastava¹³ concluded that the corresponding multichannel eikonal treatment provided the best agreement with their recent measurements.

Cross sections obtained for the corresponding triplet-triplet transitions are smaller than and demonstrate behavior similar to that in Fig. 5, and are available from the authors, upon request.

Angular-Correlation Parameters and Circular Polarization Fractions.

In Figs. (6a, b) are presented graphical displays, as functions of θ and E, of λ , the relative contribution to the differential cross section arising from $1^1P(m=0)$ scattering, and of χ , the phase difference between the 1^1P -dipoles oscillating ($m=0$) and rotating ($m=\pm 1$) about the Z-axis. Forward ($\theta \approx 0$) and large-angle ($\theta \geq 40^\circ$) inelastic scattering is mainly in the $m=0$ channel, with $m=\pm 1$ excitations being dominant at the intermediate angles. As E is decreased, this intermediate angular range increases and the range for $m=0$ scattering in the forward direction also

increases, although not as rapidly.

The 2^1P phase difference χ_1 in Fig. (5b) is negative for all θ and passes through $(-\frac{\pi}{2})$ twice for all E , and $(-\pi)$ twice only for the lowest $E \sim 5\text{eV}$. This behavior assumes significance in the fraction of circularly polarized radiation emitted from the 2^1P states. Thus, provided the populations of the $m=0$ and ± 1 sublevels are equal (i.e. $\lambda \approx 0.5$), then $\Pi = -\sin\chi$ and fully circularly polarized light is observed when $\chi \approx -\pi/2$ and is absent when $\chi \approx -\pi$ at two scattering angles θ . Fig. (5a) however shows that the $m=0$ and $m=\pm 1$ substates are not equally populated, in general, except at specific θ , and the combined effect of phase difference and departure from equal populations is exhibited in Fig. (6) which displays Π given by (17) as a function of θ and E . This figure shows that circularly polarized light is observed when the electrons are scattered through fairly large angles which decrease as E increases. Moreover, Π passes through zero twice, only for $E = 0.5\text{ eV}$, as expected from Fig. (5b). Fig. (7) also provides the angular momentum (17) transferred at right angles to the scattering plane, and hence the maxima, almost reaching unity, correspond to the transfer of ~ 1 unit of angular momentum (\hbar) to the atom which is therefore left in the $m = 0$ state.

Similar graphical displays of λ , χ and Π have been obtained for the remaining transitions (and are available from the authors). No experimental data exist. However, a corresponding ten-channel treatment⁴ of the $1^1S - 2^1P$, 3^1P transitions in helium by electron-impact resulted in satisfactory agreement with the recent λ , χ -measurements of Eminyan et al.⁸

We note that a fully quantal close-coupling calculation would in practice be prohibitively difficult in that an extremely large number of angular momentum states L of relative motion are distorted by the strong dipole interactions evident in the present study. Thus the normal procedure of performing fully quantal computations for $L = 0 \rightarrow L_{\max} \sim 10$, and a Born approximation for $L > 10$ simply will not suffice since the present investigation has shown that impact parameters $\rho \sim 100$ a.u. ($\equiv L/k_i$) are influenced appreciably by the various distortions. The advantage of the present treatment is that the multichannel eikonal expansion (5) ensures that convergence in partial wave contributions is always attained especially in the high-energy limit without undue difficulty and that the long-range couplings have a mechanism whereby they can affect distant encounters (or large L) important to the processes investigated here.

Finally, the effect of the neglect of electron-exchange and of couplings with channels $n \geq 4$ is difficult to assess, without resort to more detailed and elaborate calculations. For transitions from the 1^1S -state, electron exchange is effective only for the close encounters resulting in large-angle scattering. These large angles, however, provide negligible contribution to the inelastic integral cross sections,^{4,14} which are determined solely by scattering mainly in the forward direction ($\theta \lesssim 20^\circ$) at intermediate impact energies. Also, explicit inclusion¹ of exchange within the the VPS-approximation for e-He($2^{1,3}S$) collisions causes little change for $E \gtrsim 10$ eV. A better representation of the direct scattering function is apparently more important and is obtained by the present inclusion of close-couplings.

In conclusion, for e-He($2^{1,3}S$) inelastic collisions at impact energies $E \leq 100$ eV, couplings with the neighboring $n = 2$ and 3 levels are important, particularly those involving the $3^{1,3}D$ states, the excitation of which dominate transitions to the $n = 3$ level at low E . The Born-limit is approached at energies (~ 100 eV for singlet-singlet transitions) lower than those normally in evidence for excitation from ground states. Detailed balance between the forward and reverse rates of the $2^1S \rightleftharpoons 1^1S$ transitions is satisfied. The competition between the relative populations λ of the magnetic P-substates and the phases χ of the corresponding excitations is exhibited by the variation of Π , the fraction of circularly polarized radiation emitted from these P-states, with impact energy E and scattering-angle θ .

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Table I. Integral cross sections (πa_0^2) for the 2^1S-n^1L and 2^3S-n^3L transitions (S and T respectively) in helium by collision with incident electrons of energy E(eV)

	S	T	S	T	S	T	S	T	S	T
E(eV) nL(m)	5		10		20		50		100	
2P(0)	5.71 ^{1a}	3.07 ¹	4.01 ¹	2.38 ¹	1.02 ¹	1.29 ¹	9.94 ⁻¹	2.26	2.58 ⁻¹	1.64
2P(± 1)	1.23 ²	4.63 ¹	1.22 ²	5.53 ¹	9.51 ¹	4.70 ¹	5.63 ¹	2.81 ¹	3.16 ¹	1.67 ¹
2P(Σ)	1.80 ²	7.70 ¹	1.62 ²	7.91 ¹	1.05 ²	5.99 ¹	5.73 ¹	3.04 ¹	3.19 ¹	1.83 ¹
3S	5.92	1.95	3.99	1.72	2.52	1.20	1.19	6.18 ⁻¹	6.29 ⁻¹	3.21 ⁻¹
3P(0)	1.08	6.42 ⁻¹	8.40 ⁻¹	3.78 ⁻¹	9.29 ⁻¹	2.38 ⁻¹	4.57 ⁻¹	2.60 ⁻¹	1.80 ⁻¹	2.00 ⁻¹
3P(± 1)	3.72 ⁻¹	9.48 ⁻²	7.36 ⁻¹	3.24 ⁻¹	1.10	3.40 ⁻¹	1.36	2.68 ⁻¹	1.02	1.80 ⁻¹
3P(Σ)	1.45	7.37 ⁻¹	1.58	7.02 ⁻¹	2.03	5.78 ⁻¹	1.82	5.28 ⁻¹	1.20	3.80 ⁻¹
3D(0)	2.73	1.34	3.03	1.72	1.49	8.34 ⁻¹	4.69 ⁻¹	2.81 ⁻¹	2.34 ⁻¹	2.17 ⁻¹
3D(± 1)	6.56	1.89	7.16	3.20	3.58	1.81	8.96 ⁻¹	6.35 ⁻¹	2.29 ⁻¹	2.51 ⁻¹
3D(± 2)	1.78	3.87 ⁻¹	3.89	1.40	3.52	1.45	1.92	8.55	1.02	5.41 ⁻¹
3D(Σ)	1.11 ¹	3.62	1.41 ¹	6.32	8.59	4.09	3.28	1.77	1.48	1.01
1 ¹ S	1.47 ⁻¹	-	8.63 ⁻²	-	5.06 ⁻²	-	2.91 ⁻²	-	1.71 ⁻²	-

a Exponents indicate the power of 10 by which the entry is to be multiplied.

Table II. Polarization fractions of radiation of wavelength

λ (Å) emitted from the collisionally excited states n' to state n .

$n'-n$ E(eV)	2^1P-n^1S	2^3P-2^3S	3^1P-n^1S	3^3P-2^3S	3^1D-2^1P	3^3D-2^3P
	$\lambda(\text{Å})$	$\lambda(\text{Å})$	$\lambda(\text{Å})$	$\lambda(\text{Å})$	$\lambda(\text{Å})$	$\lambda(\text{Å})$
	20,581(2) ^a	10,830	5016(2)	3889	6678	5876
	584(1)		537(1)			
5	-0.037	0.040	0.706	0.302	0.262	0.175
10	-0.207	-0.020	0.391	0.123	0.138	0.104
20	-0.647	-0.076	0.256	0.048	-0.021	0.025
50	-0.932	-0.171	-0.196	0.096	-0.248	-0.052
100	-0.968	-0.161	-0.478	0.116	-0.383	-0.072

^aValue of lower-level n in parenthesis.

FIGURE CAPTIONS

- Fig. 1. Cross sections (πa_0^2) for the $2^{1,3}S-2^{1,3}P$ transitions induced in helium by electron-impact at energy $E(\text{eV})$.
 E: Present multichannel eikonal treatment.
 B: Born Approximation.^{1,10}
 C: Burke et al.¹¹
- Fig. 2. Cross sections (πa_0^2) for the 2^1S-3^1S , 3^1P , 3^1D transitions induced in helium by electron-impact at energy $E(\text{eV})$.
 E: Present treatment.
 B: Born Approximation.^{1,10}
- Fig. 3. Cross sections (πa_0^2) for the 2^3S-3^3S , 3^3P , 3^3D transitions induced in helium by electron-impact at energy $E(\text{eV})$.
 E: Present treatment.
 B: Born Approximation.^{1,10}
- Fig. 4. Test of detailed balance between the forward and reverse rates of the 1^1S-2^1S collisional excitation in helium by electrons with wavenumber k_G and k_E in the 1^1S and 2^1S channels, respectively.
 ● : Previous $\sigma(1^1S-2^1S)$ data.⁴
 X : Present $\sigma(2^1S-1^1S)$ data.
- Fig. 5. Differential cross sections ($a_0^2/\text{sterad.}$) as a function of scattering angle $\theta(\text{deg})$ and impact-energy $E(\text{eV})$ indicated on each curve for (a) 2^1P , (b) 3^1S , (c) 3^1P and (d) 3^1D excitations, summed over final magnetic substates m .
- Fig. 6. Variation of (a) $\lambda(2^1P)$ and (b) $\chi(2^1P)$ with electron-scattering angle $\theta(\text{deg})$ and with electron-impact-energy $E(\text{eV})$ indicated on each curve.
- Fig. 7. The variation of the fraction Π of circularly polarized radiation, emitted from $\text{He}(2^1P)$ and observed perpendicular to the scattering plane, with electron-scattering angle θ and impact-energy $E(\text{eV})$ indicated on each curve.

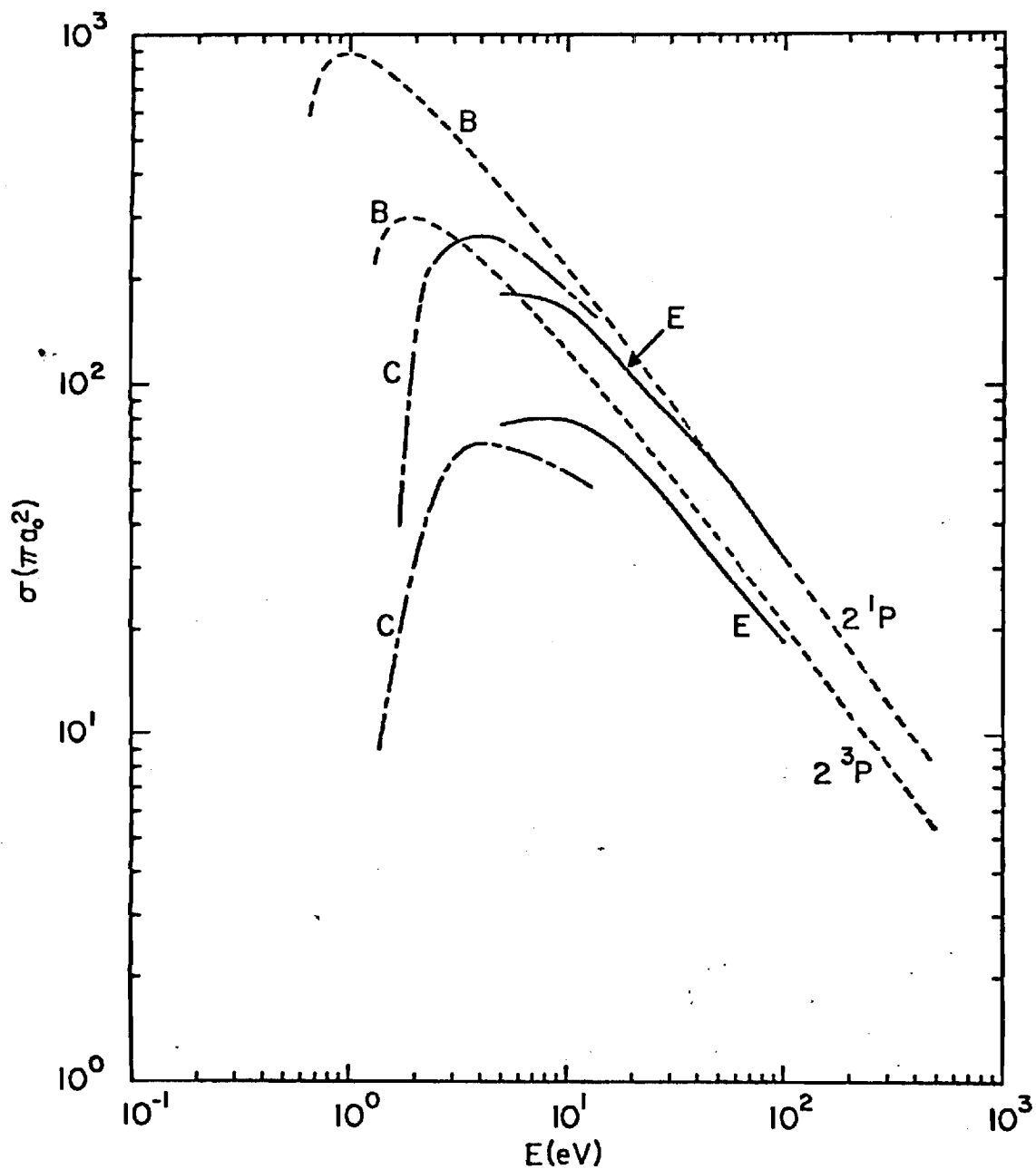


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 C: Burke et al.¹¹

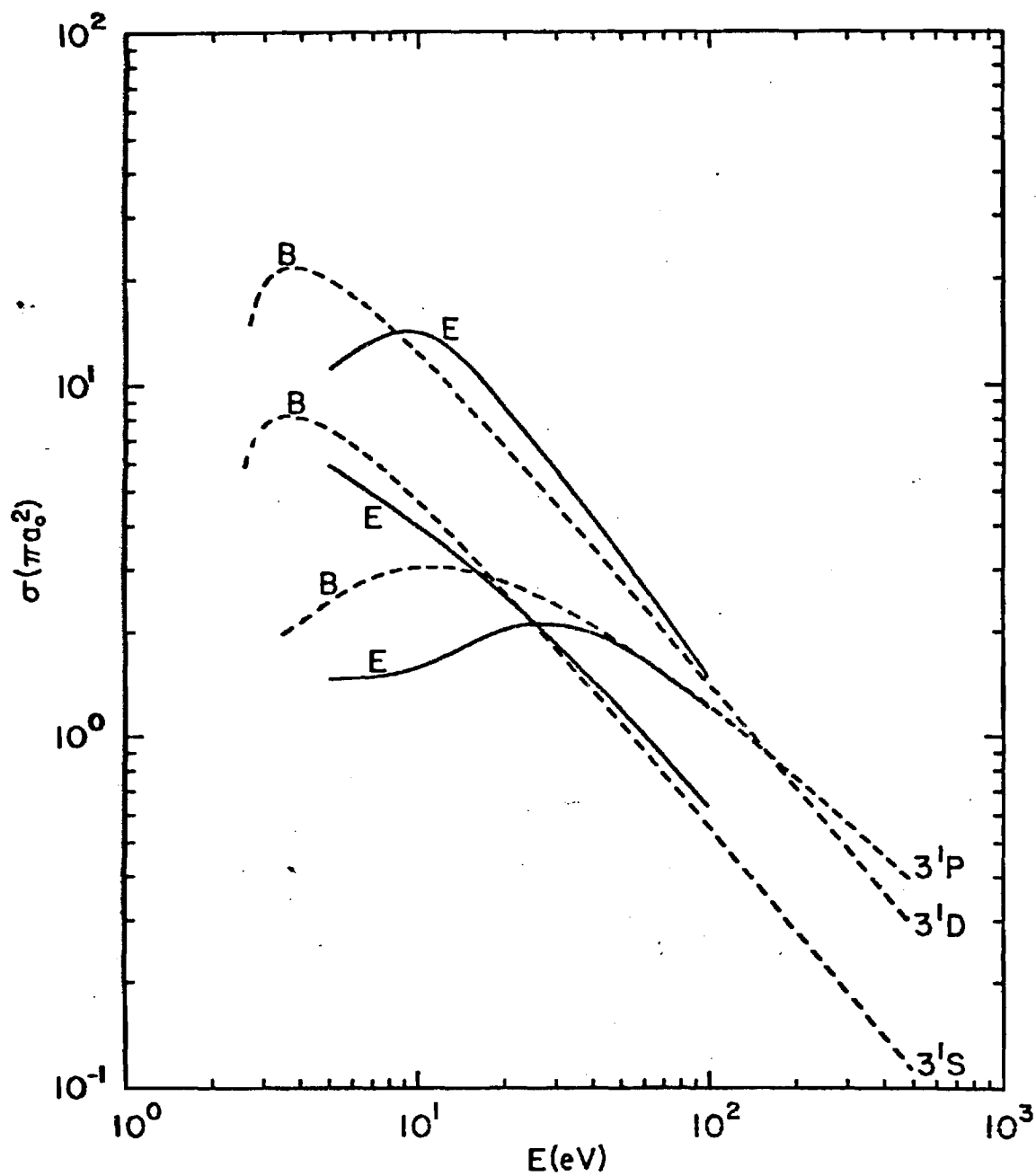


Fig. 2. Cross sections (πa_0^2) for the 2^1S-3^1S , 3^1P , 3^1D transitions induced in helium by electron-impact at energy $E(\text{eV})$.

E: Present treatment.

B: Born Approximation.^{1, 10}

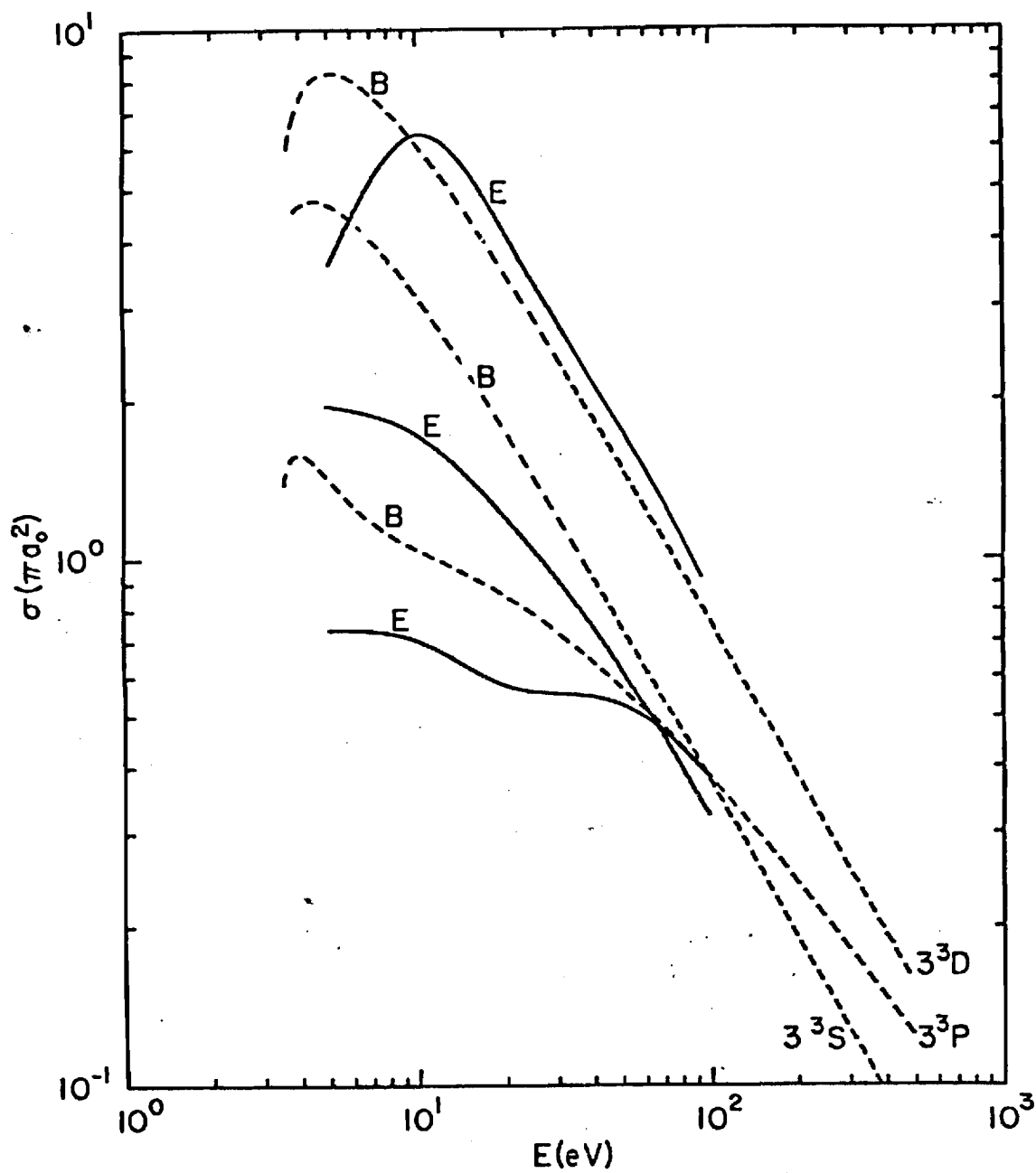


Fig. 3. Cross sections (πa_0^2) for the 2^3S - 3^3S , 3^3P , 3^3D transitions induced in helium by electron-impact at energy $E(\text{eV})$.
 E: Present treatment.
 B: Born Approximation.^{1, 10}

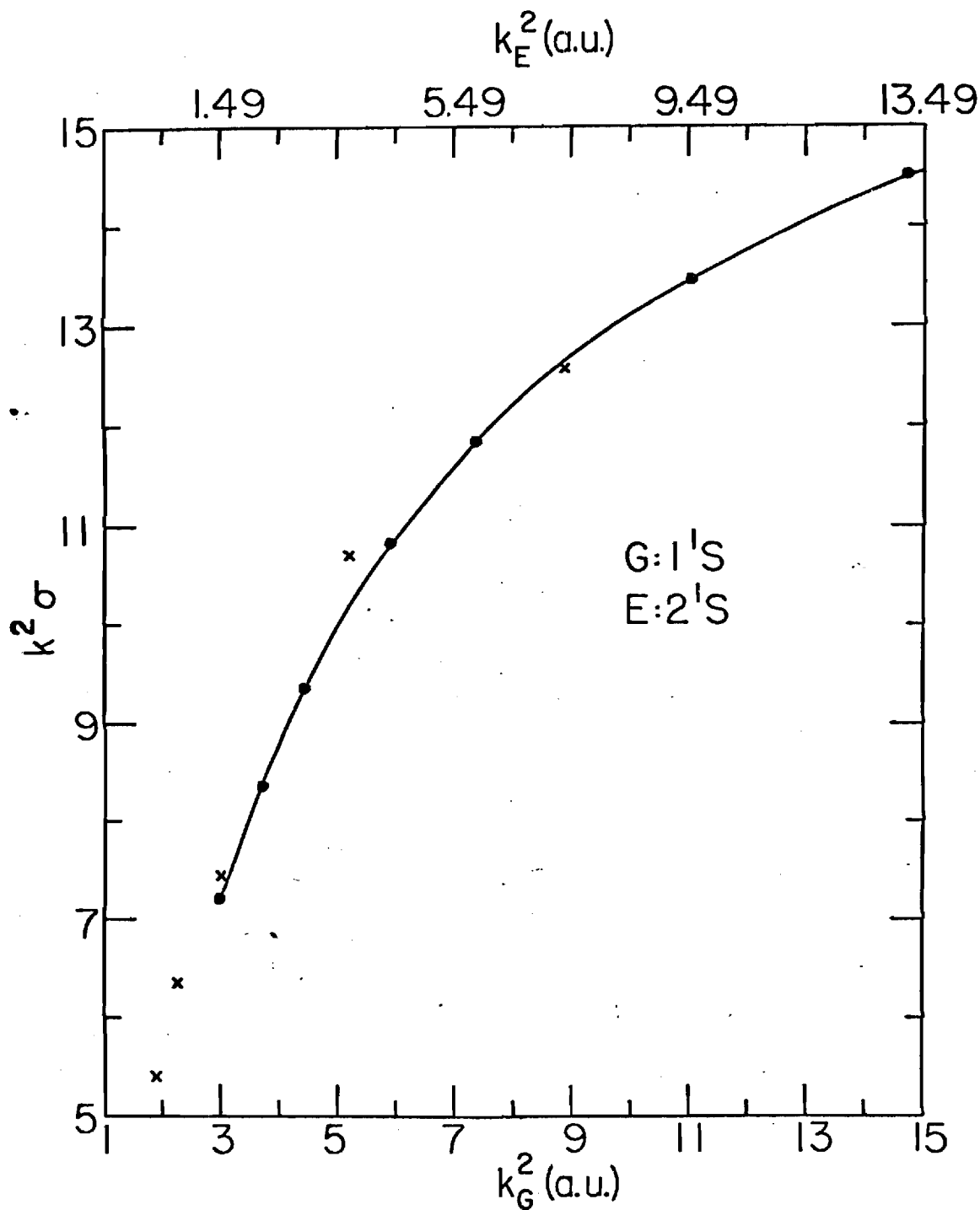


Fig. 4. Test of detailed balance between the forward and reverse rates of the 1^1S - 2^1S collisional excitation in helium by electrons with wavenumber k_G and k_E in the 1^1S and 2^1S channels, respectively.

● : Previous $\sigma(1^1S - 2^1S)$ data.⁴

× : Present $\sigma(2^1S - 1^1S)$ data.

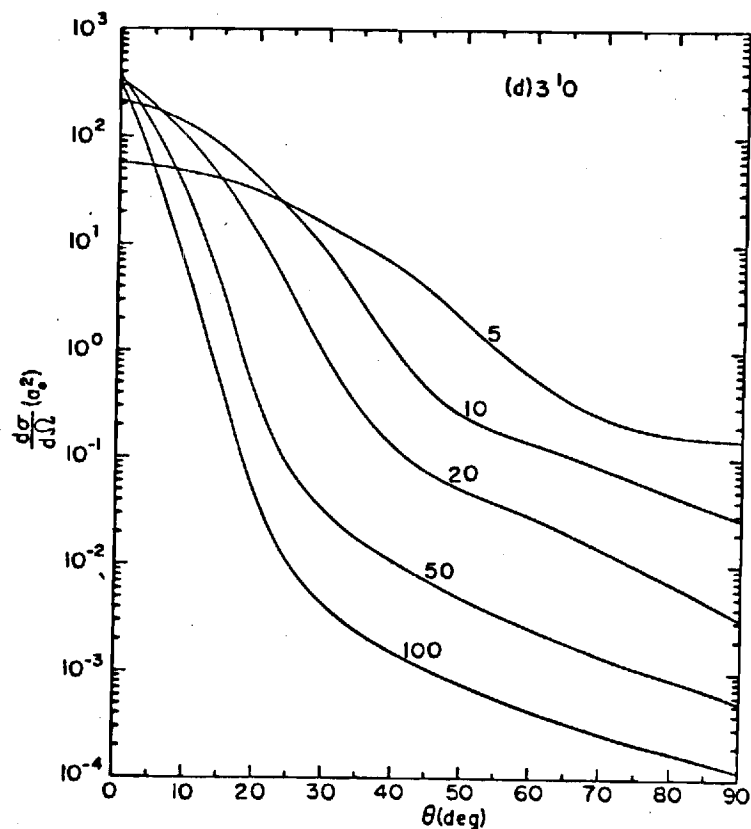
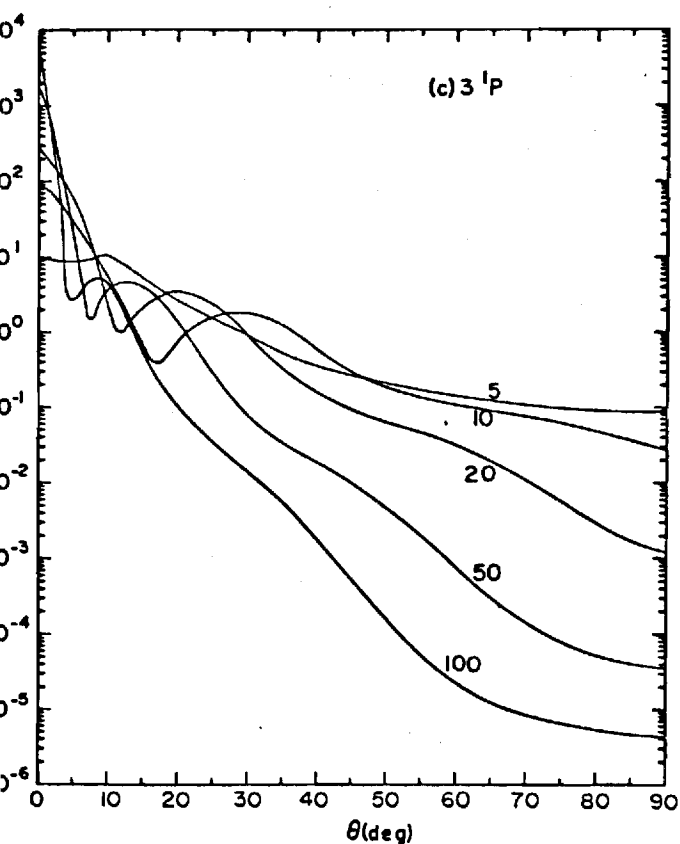
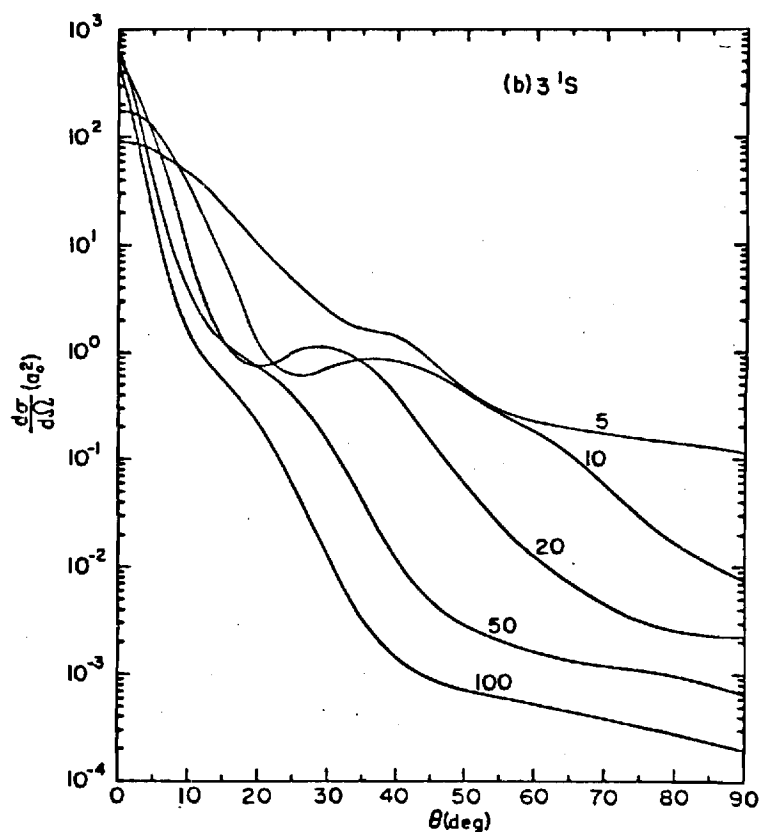
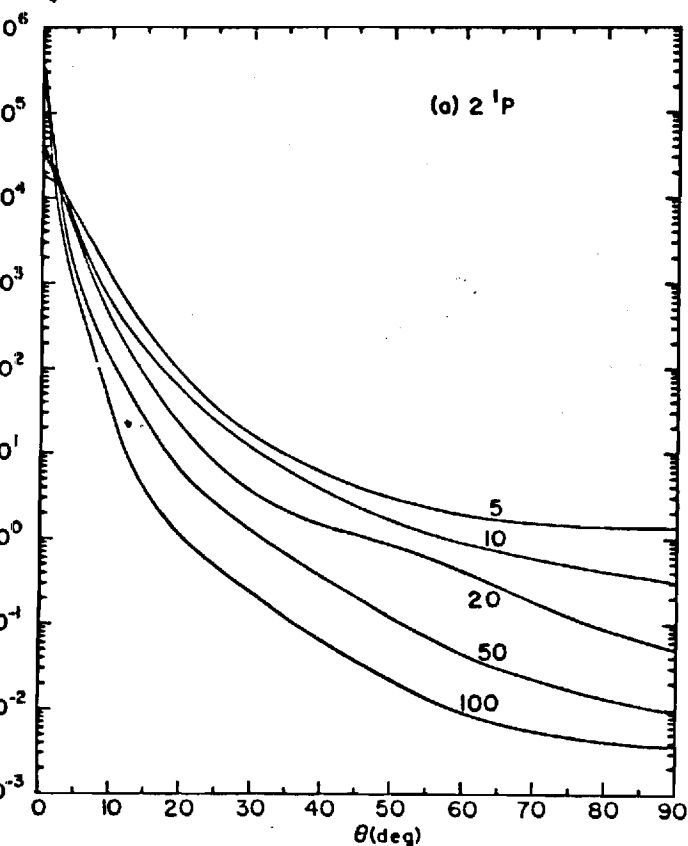


Fig. 5. Differential cross sections ($a_0^2/\text{sterad.}$) as a function of scattering angle $\theta(\text{deg})$ and impact-energy $E(\text{eV})$ indicated on each curve for (a) 2^1P , (b) 3^1S , (c) 3^1P and (d) 3^1D excitations, summed over final magnetic substates m .

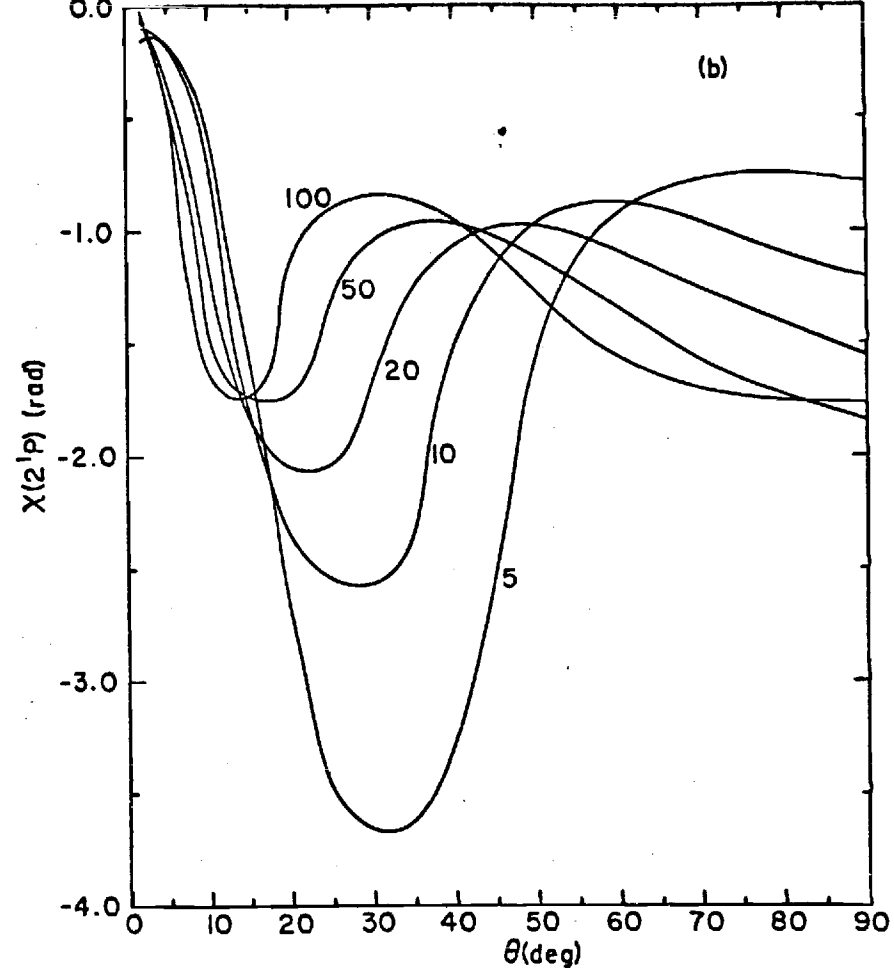
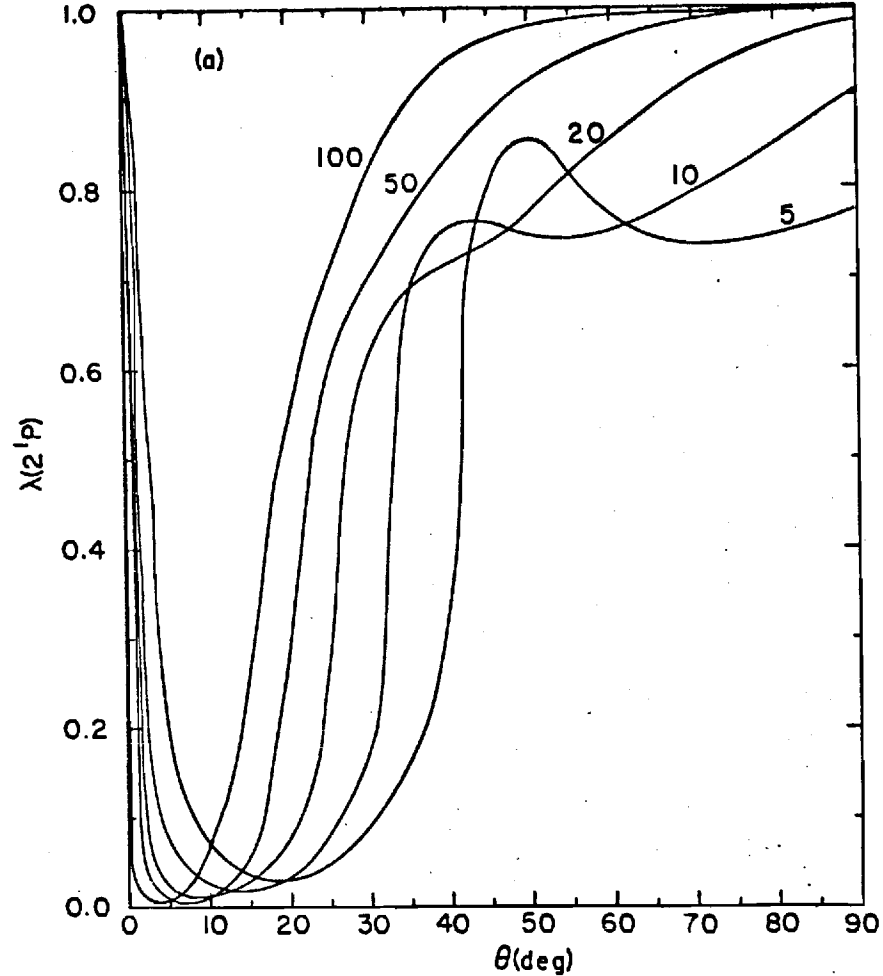


Fig. 6. Variation of (a) $\lambda(2^1P)$ and (b) $\chi(2^1P)$ with electron-scattering angle $\theta(\text{deg})$ and with electron-impact-energy $E(\text{eV})$ indicated on each curve.

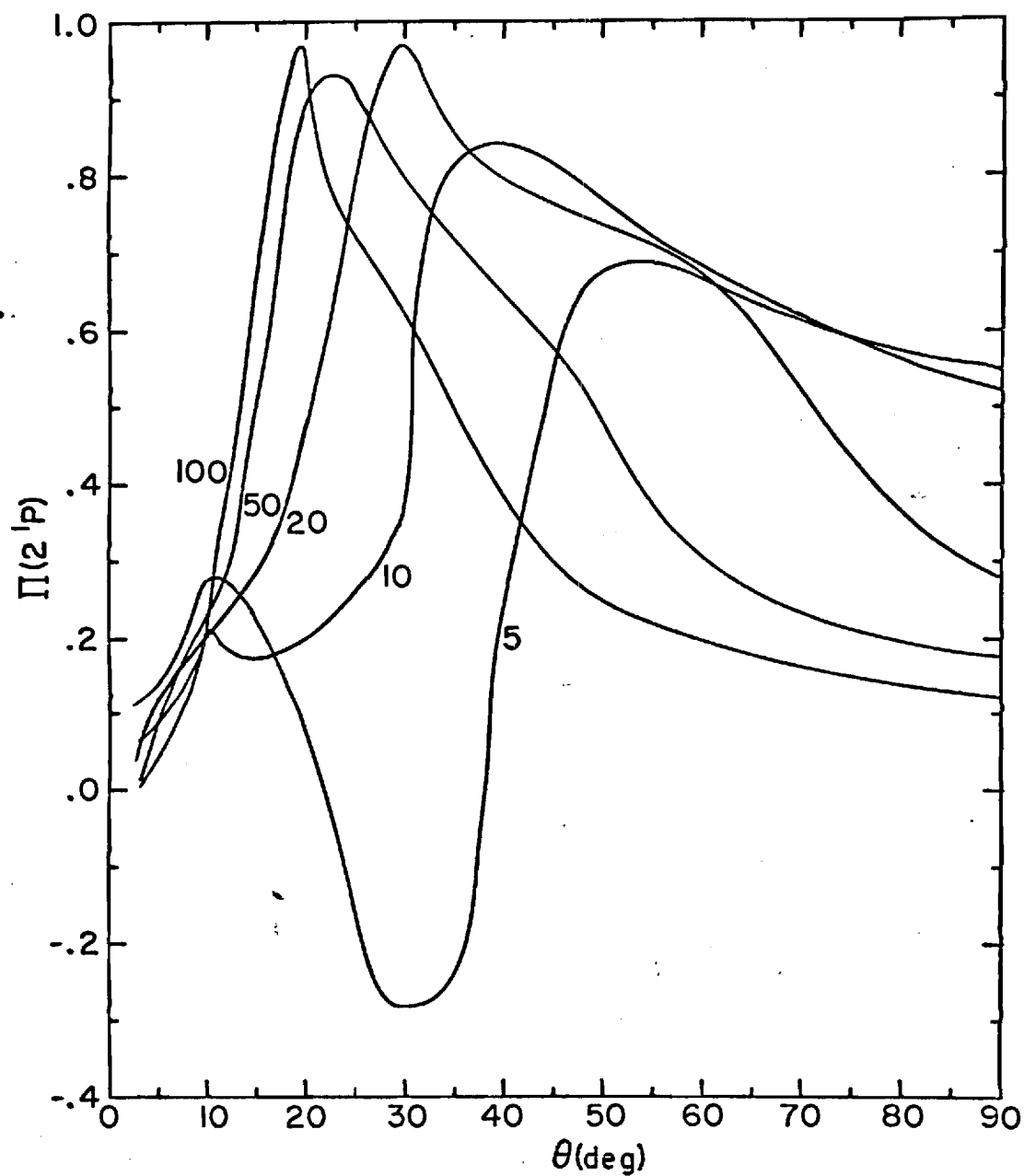


Fig. 7. The variation of the fraction Π of circularly polarized radiation, emitted from $\text{He}(2^1P)$ and observed perpendicular to the scattering plane, with electron-scattering angle θ and impact-energy $E(\text{eV})$ indicated on each curve.